



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:17 AM UTC

PDB ID : 8Q45 / pdb_00008q45
EMDB ID : EMD-18138
Title : Inward-facing, closed proteoliposome complex I at 2.7 Å. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-05
Resolution : 2.70 Å(reported)
Based on initial model : 7QSN

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

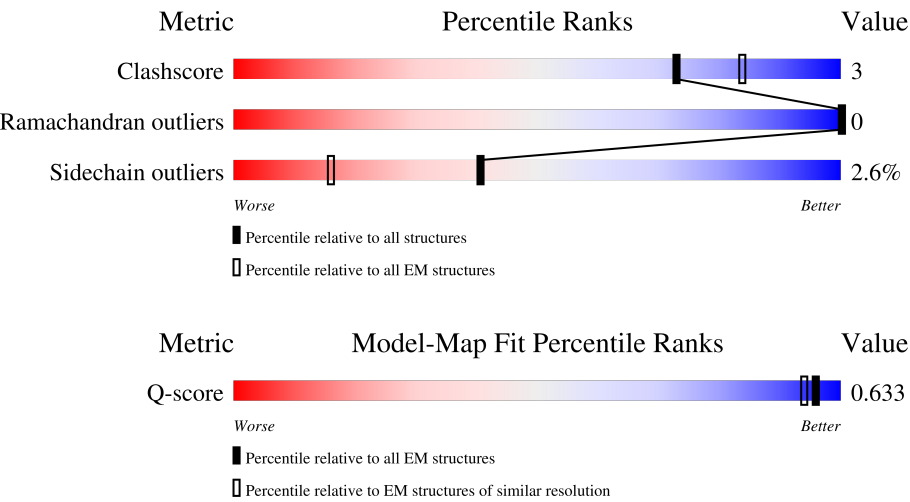
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



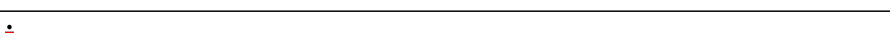
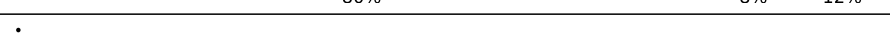
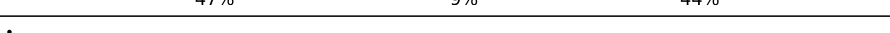
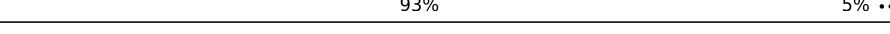
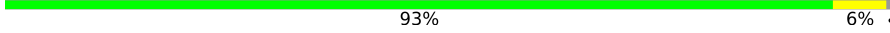
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	87%12%.
2	B	216	62%9%28%
3	C	266	73%5%21%
4	D	463	85%8%7%

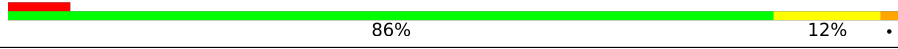
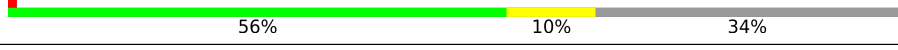
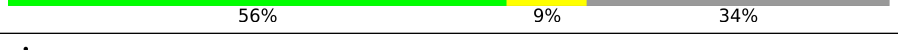
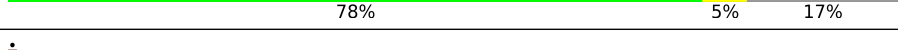
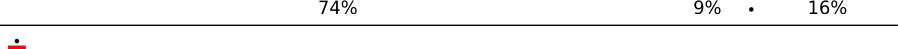
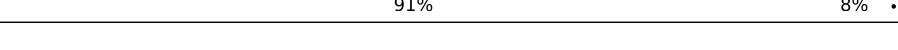
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
49	U10	D	501	-	-	X	-

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 70020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1738	1120	298	317	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	0	0
			3326	2096	594	616	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	695	Total	C	N	O	S	0	0
			5325	3335	929	1021	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2754	1781	487	481	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			707	454	104	144	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			976	625	181	166	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			654	427	109	116	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	99	Total	C	N	O	S	0	0
			829	523	158	142	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			846	544	140	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	127	Total	C	N	O	S	0	0
			1097	722	191	183	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	128	Total	C	N	O	S	0	0
			1070	686	188	196			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	174	Total	C	N	O	S	0	0
			1458	913	269	268	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1212	780	216	211	5		

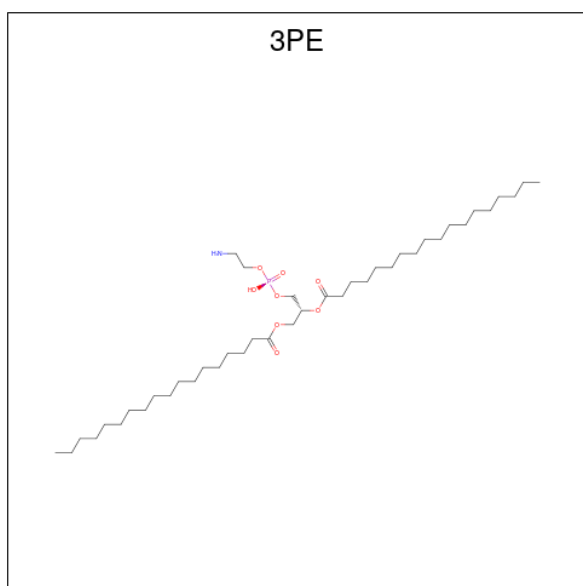
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			776	490	144	139	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	45	Total	C	N	O	S	0	0
			380	238	67	74	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	I	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	J	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	J	1	Total	C	N	O	P	0
			35	25	1	8	1	

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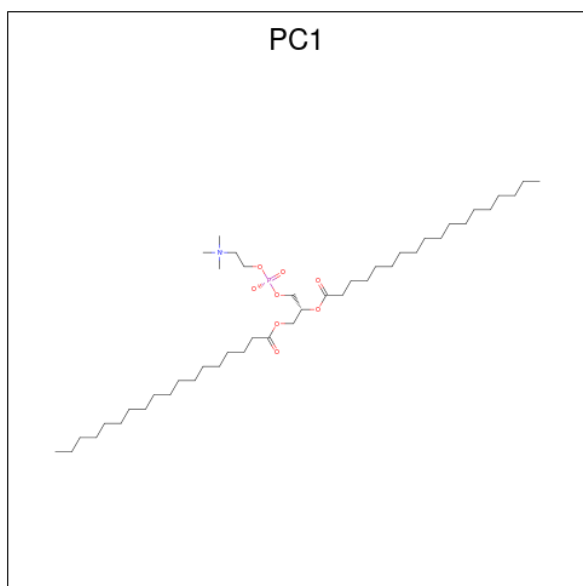
Mol	Chain	Residues	Atoms					AltConf
45	J	1	Total 44	C 34	N 1	O 8	P 1	0
45	L	1	Total 45	C 35	N 1	O 8	P 1	0
45	L	1	Total 34	C 24	N 1	O 8	P 1	0
45	L	1	Total 51	C 41	N 1	O 8	P 1	0
45	M	1	Total 50	C 40	N 1	O 8	P 1	0
45	N	1	Total 49	C 39	N 1	O 8	P 1	0
45	P	1	Total 35	C 25	N 1	O 8	P 1	0
45	P	1	Total 32	C 22	N 1	O 8	P 1	0
45	Y	1	Total 45	C 35	N 1	O 8	P 1	0
45	Y	1	Total 23	C 13	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 39	C 29	N 1	O 8	P 1	0
45	Y	1	Total 47	C 37	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Z	1	Total 42	C 32	N 1	O 8	P 1	0
45	a	1	Total 36	C 26	N 1	O 8	P 1	0
45	b	1	Total 51	C 41	N 1	O 8	P 1	0
45	d	1	Total 49	C 39	N 1	O 8	P 1	0
45	g	1	Total 40	C 30	N 1	O 8	P 1	0
45	j	1	Total 40	C 30	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
45	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	m	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	p	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	q	1	Total	C	N	O	P	0
			21	11	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



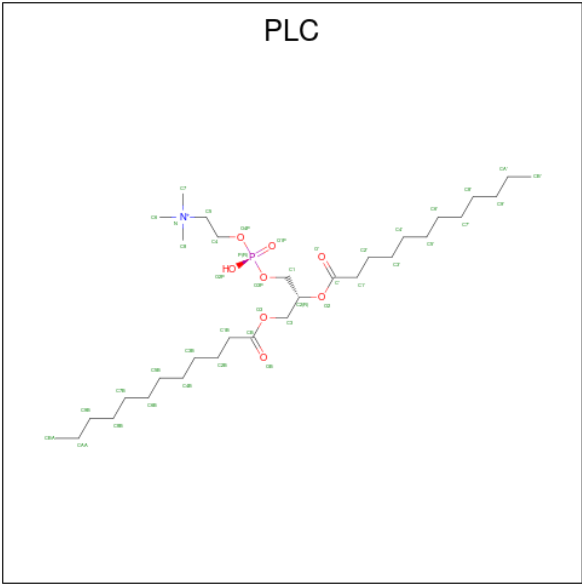
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	I	1	Total	C	N	O	P	0
			44	34	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	P	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	g	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	h	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	q	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 47 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



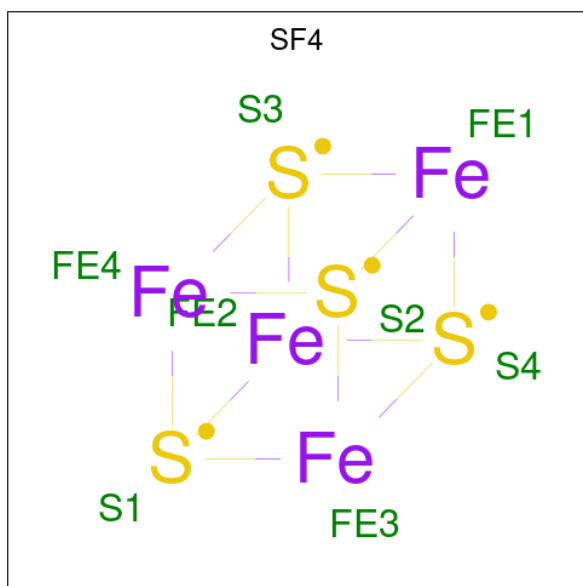
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
47	B	1	Total	C	N	O	P	0
			37	27	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
47	J	1	Total	C	N	O	P	0
			38	28	1	8	1	
47	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	O	1	Total	C	N	O	P	0
			32	22	1	8	1	
47	P	1	Total	C	N	O	P	0
			27	17	1	8	1	
47	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	d	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	h	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



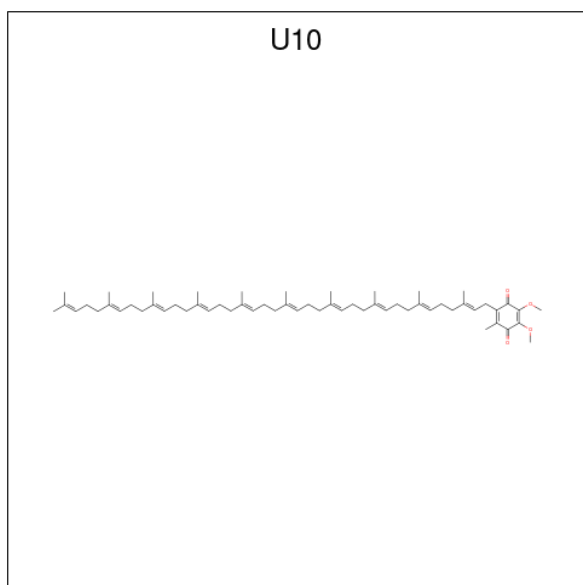
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	

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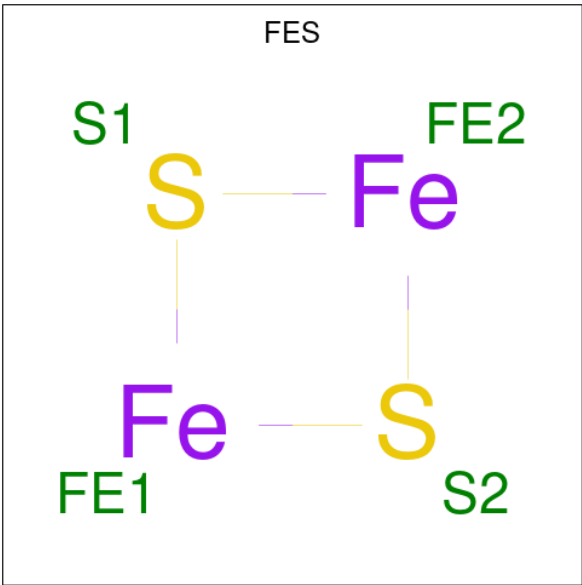
Mol	Chain	Residues	Atoms			AltConf
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



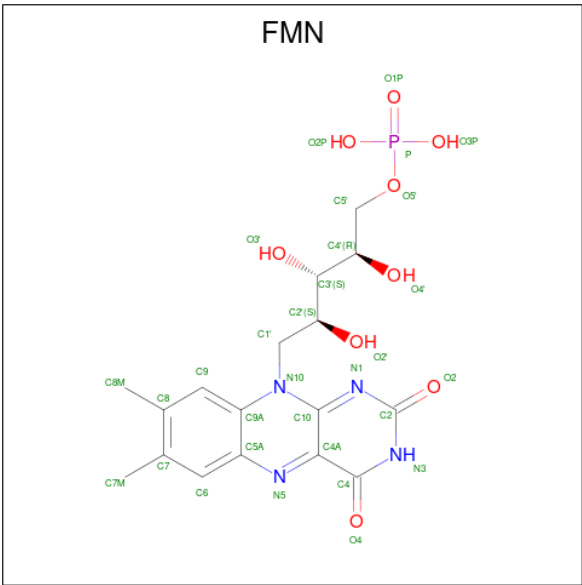
Mol	Chain	Residues	Atoms			AltConf
49	D	1	Total	C	O	0
			63	59	4	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
50	E	1	Total	Fe	S	0
			4	2	2	
50	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 51 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

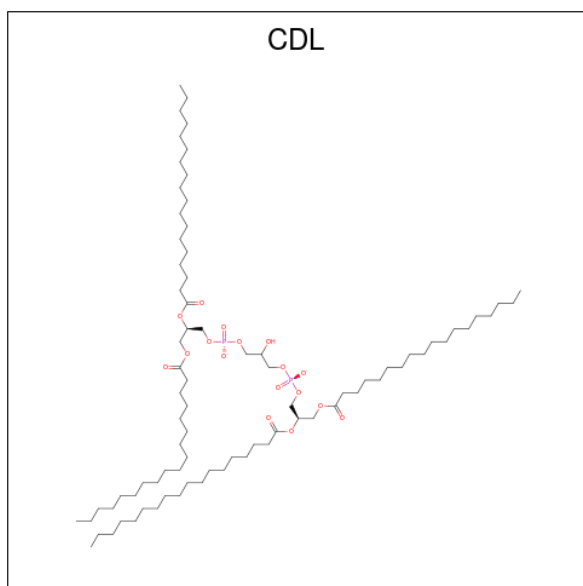


Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
52	G	1	Total	K	0
			1	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

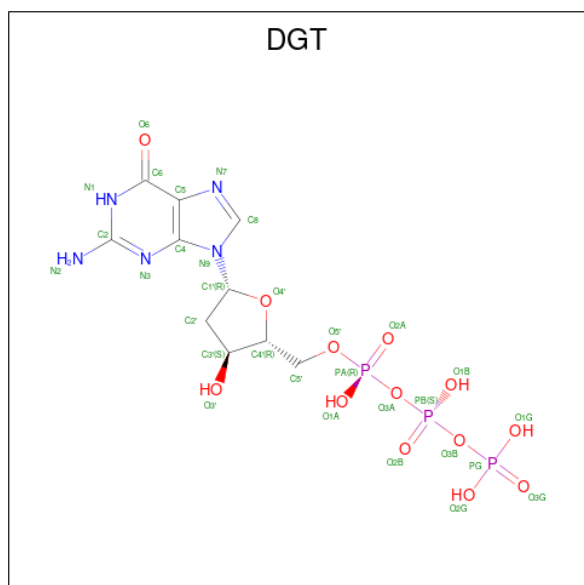


Mol	Chain	Residues	Atoms				AltConf
53	J	1	Total	C	O	P	0
			70	51	17	2	
53	L	1	Total	C	O	P	0
			76	57	17	2	
53	M	1	Total	C	O	P	0
			100	81	17	2	
53	N	1	Total	C	O	P	0
			80	61	17	2	
53	P	1	Total	C	O	P	0
			83	64	17	2	
53	X	1	Total	C	O	P	0
			100	81	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	i	1	Total	C	O	P	0
			80	61	17	2	
53	q	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	M	1	Total	Zn	0
			1	1	
54	R	1	Total	Zn	0
			1	1	

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	O	1	Total	Mg	0
			1	1	

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



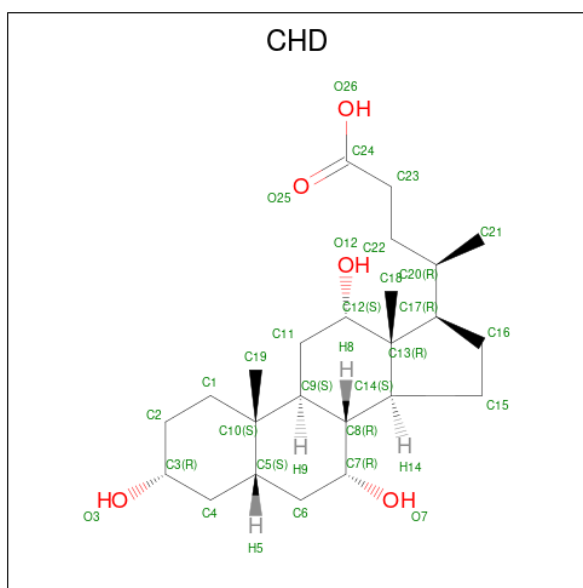
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



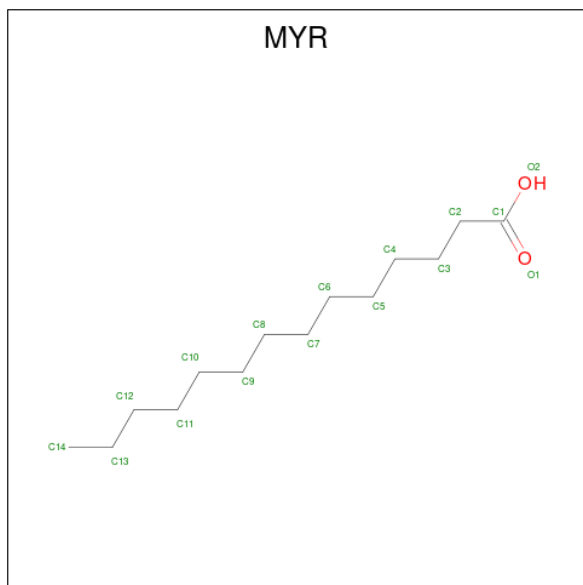
Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total 37	C 25	N 2	O 8	P 1	S 1	0
58	U	1	Total 37	C 25	N 2	O 8	P 1	S 1	0

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			AltConf
59	i	1	Total	C	O	0
			29	24	5	

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

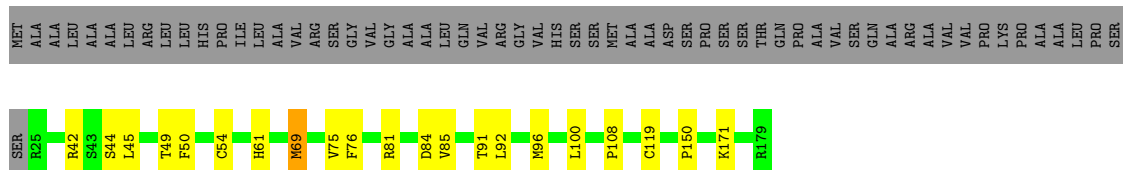
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



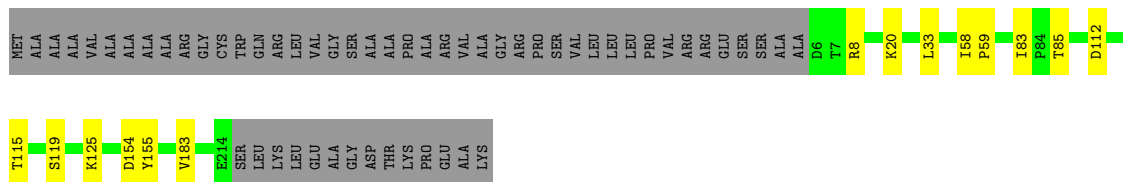
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



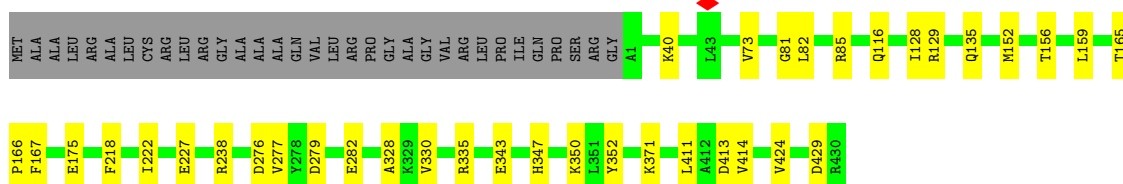
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



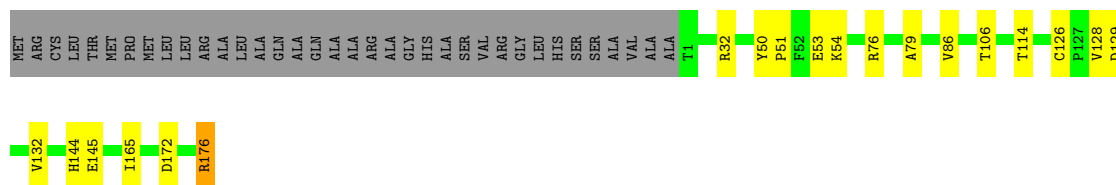
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  74% 8% 17%



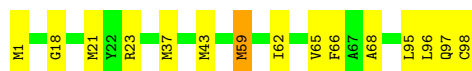
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  89% 10%



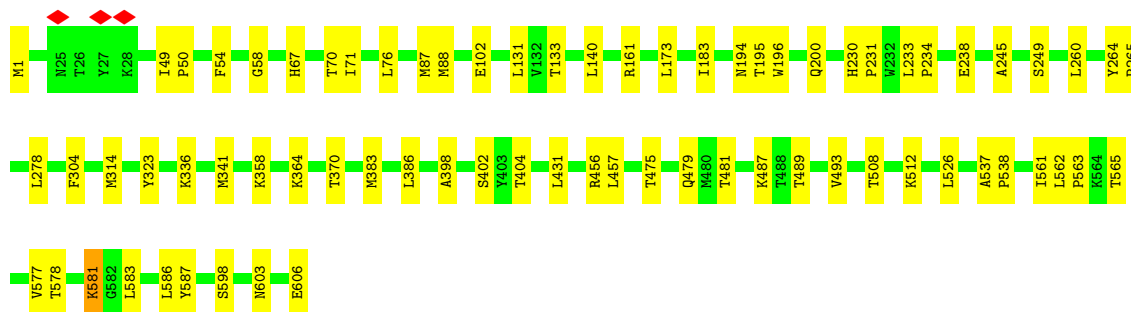
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  85% 14%



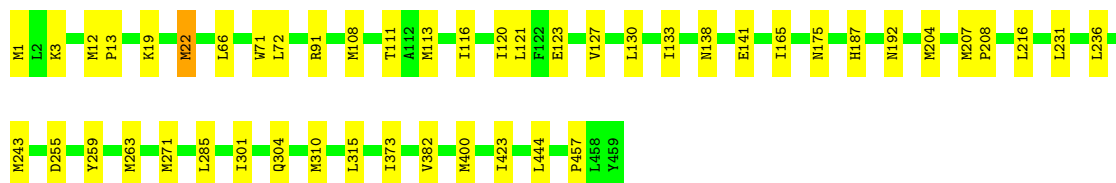
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  88% 12%



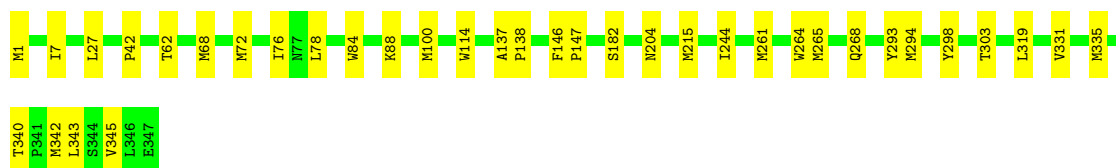
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  90% 10%



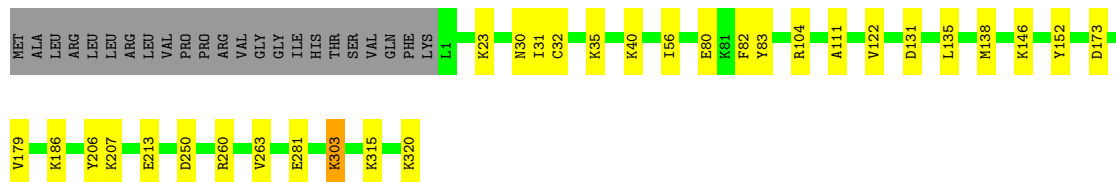
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  90% 10%



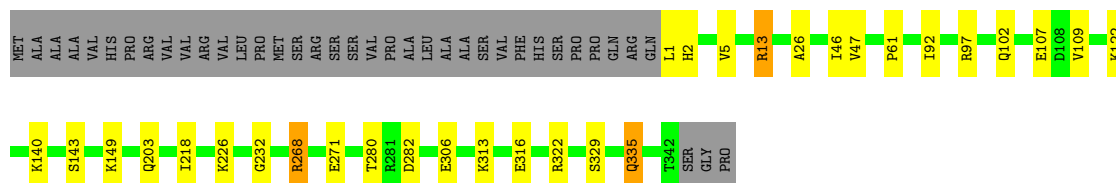
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 84% 9% 7%



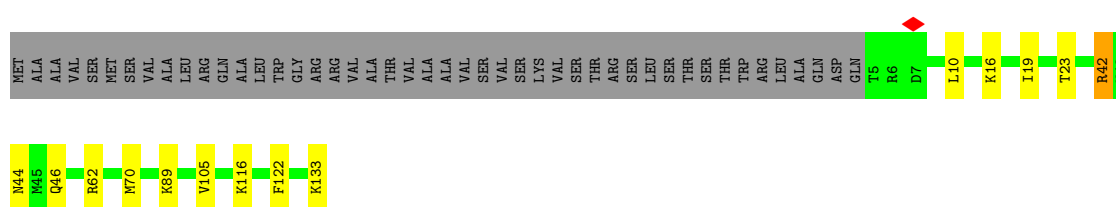
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 82% 7% 10%



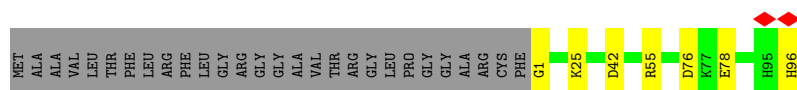
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 66% 7% 26%



- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 72% 6% 23%

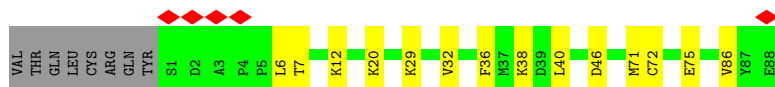


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S: 80% 8% 12%



- Molecule 20: Acyl carrier protein, mitochondrial



- Molecule 20: Acyl carrier protein, mitochondrial



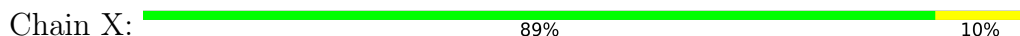
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

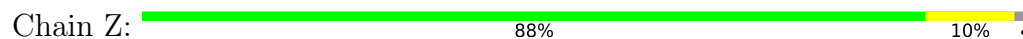


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

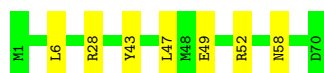
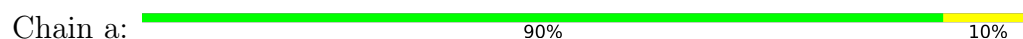




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



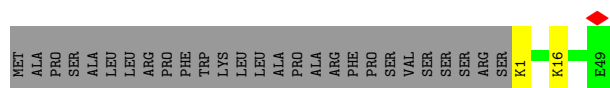
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



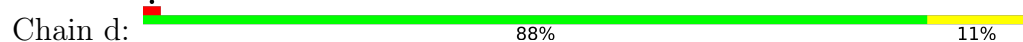
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



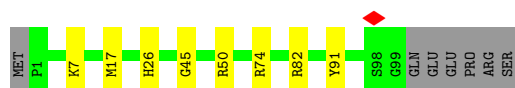
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



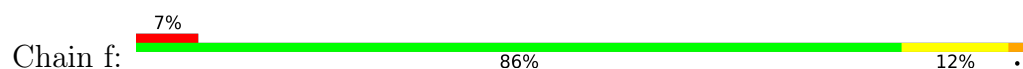
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

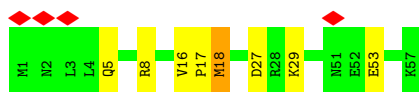


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

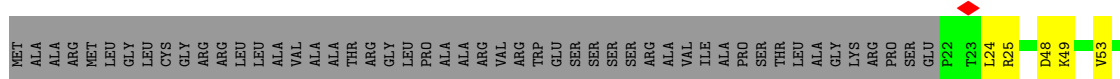


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

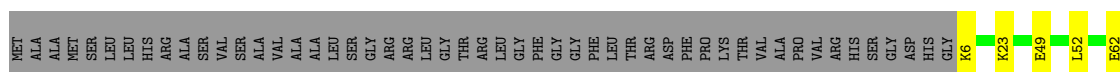




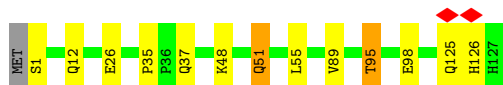
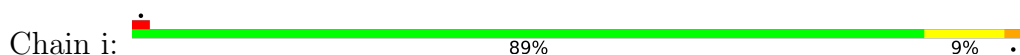
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



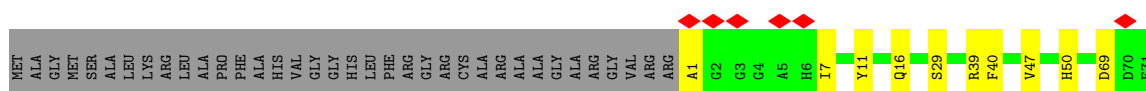
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



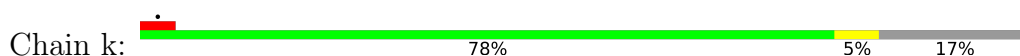
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

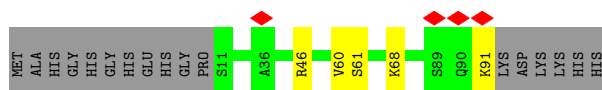


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3





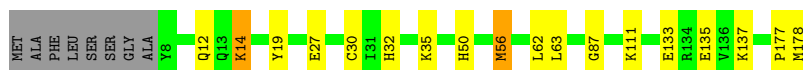
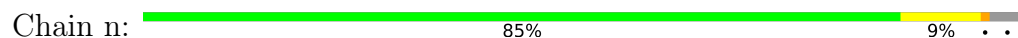
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



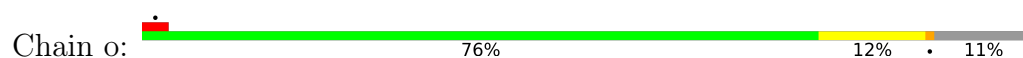
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



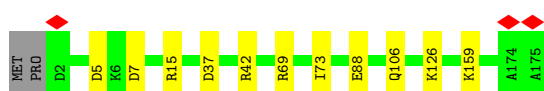
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



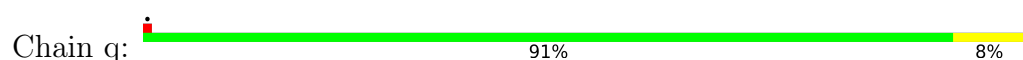
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

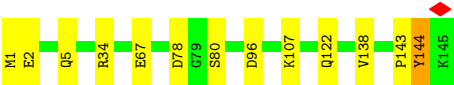


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

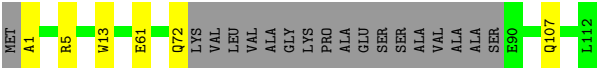
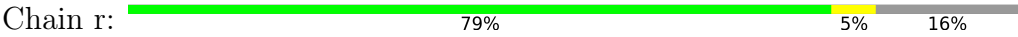


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

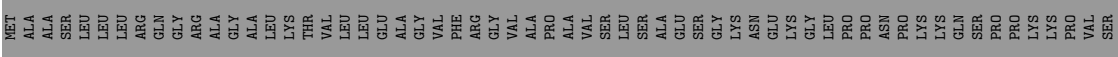




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63569	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.297	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	479.69998, 479.69998, 479.69998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MYR, AME, MG, 3PE, PC1, SAC, ZN, NDP, EHZ, DGT, CDL, SF4, FMN, 2MR, CHD, PLC, AYA, FES, FME, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/936	0.22	0/1281
2	B	0.12	0/1272	0.25	0/1720
3	C	0.12	0/1789	0.26	0/2436
4	D	0.12	0/3537	0.23	0/4794
5	E	0.10	0/1699	0.25	0/2312
6	F	0.10	0/3401	0.23	0/4595
7	G	0.10	0/5414	0.24	0/7336
8	H	0.12	0/2571	0.26	0/3513
9	I	0.13	0/1445	0.25	0/1956
10	J	0.11	0/1370	0.22	0/1859
11	K	0.11	0/745	0.23	0/1008
12	L	0.10	0/4920	0.24	0/6694
13	M	0.11	0/3738	0.23	0/5097
14	N	0.11	0/2792	0.23	0/3800
15	O	0.10	0/2651	0.22	0/3587
16	P	0.11	0/2831	0.23	0/3841
17	Q	0.11	0/1072	0.23	0/1449
18	R	0.13	0/753	0.20	0/1014
19	S	0.08	0/711	0.22	0/956
20	T	0.10	0/719	0.21	0/971
20	U	0.11	0/719	0.22	0/971
21	V	0.11	0/948	0.20	0/1284
22	W	0.09	0/1000	0.21	0/1344
23	X	0.10	0/1439	0.23	0/1942
24	Y	0.08	0/1042	0.18	0/1414
25	Z	0.10	0/1181	0.20	0/1592
26	a	0.12	0/584	0.23	0/786
27	b	0.09	0/667	0.24	0/916
28	c	0.12	0/427	0.18	0/579
29	d	0.11	0/1018	0.25	0/1375
30	e	0.10	0/850	0.21	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.11	0/505	0.25	0/681
32	g	0.10	0/873	0.23	0/1186
33	h	0.09	0/1188	0.23	0/1607
34	i	0.09	0/1127	0.23	0/1534
35	j	0.11	0/624	0.20	0/855
36	k	0.07	0/672	0.22	0/906
37	l	0.09	0/1369	0.22	0/1873
38	m	0.09	0/1088	0.19	0/1472
39	n	0.08	0/1540	0.20	0/2085
40	o	0.11	0/1073	0.19	0/1437
41	p	0.08	0/1491	0.20	0/2011
42	q	0.11	0/1242	0.22	0/1688
43	r	0.10	0/789	0.23	0/1068
44	s	0.08	0/392	0.22	0/531
All	All	0.10	0/68214	0.23	0/92492

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	10	0
2	B	1241	0	1251	17	0
3	C	1738	0	1685	11	0
4	D	3459	0	3404	28	0
5	E	1659	0	1664	13	0
6	F	3326	0	3282	35	0
7	G	5325	0	5344	41	0
8	H	2509	0	2621	30	0
9	I	1414	0	1370	13	0
10	J	1345	0	1352	18	0
11	K	745	0	785	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	44	0
13	M	3654	0	3852	32	0
14	N	2733	0	2912	29	0
15	O	2589	0	2565	18	0
16	P	2754	0	2773	12	0
17	Q	1049	0	1045	6	0
18	R	740	0	714	3	0
19	S	700	0	719	4	0
20	T	707	0	700	4	0
20	U	707	0	700	5	0
21	V	928	0	972	5	0
22	W	976	0	991	5	0
23	X	1402	0	1379	12	0
24	Y	1030	0	1039	8	0
25	Z	1152	0	1151	12	0
26	a	569	0	568	6	0
27	b	654	0	663	3	0
28	c	414	0	415	0	0
29	d	999	0	988	10	0
30	e	829	0	829	8	0
31	f	492	0	501	5	0
32	g	846	0	798	10	0
33	h	1154	0	1168	5	0
34	i	1097	0	1108	7	0
35	j	597	0	536	5	0
36	k	653	0	639	3	0
37	l	1314	0	1210	12	0
38	m	1070	0	1068	6	0
39	n	1487	0	1433	11	0
40	o	1048	0	1016	9	0
41	p	1458	0	1430	6	0
42	q	1212	0	1183	6	0
43	r	776	0	782	4	0
44	s	380	0	349	5	0
45	A	129	0	189	0	0
45	H	41	0	59	0	0
45	I	38	0	53	0	0
45	J	110	0	145	1	0
45	L	130	0	191	1	0
45	M	50	0	77	1	0
45	N	49	0	75	0	0
45	P	67	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Y	307	0	456	2	0
45	Z	42	0	61	0	0
45	a	36	0	49	1	0
45	b	51	0	82	0	0
45	d	49	0	75	0	0
45	g	40	0	57	0	0
45	j	40	0	54	0	0
45	m	83	0	120	1	0
45	p	35	0	47	0	0
45	q	21	0	16	0	0
46	A	68	0	84	1	0
46	B	48	0	70	1	0
46	H	87	0	128	1	0
46	I	98	0	150	1	0
46	J	35	0	44	0	0
46	L	90	0	134	1	0
46	M	35	0	44	0	0
46	P	46	0	66	0	0
46	d	39	0	52	0	0
46	g	44	0	65	1	0
46	h	47	0	71	0	0
46	q	38	0	53	0	0
47	A	38	0	53	1	0
47	B	37	0	51	0	0
47	J	38	0	53	0	0
47	L	31	0	36	0	0
47	O	32	0	41	1	0
47	P	27	0	28	1	0
47	Y	36	0	49	0	0
47	d	36	0	49	0	0
47	h	32	0	41	0	0
48	B	8	0	0	1	0
48	F	8	0	0	0	0
48	G	16	0	0	0	0
48	I	16	0	0	0	0
49	D	63	0	90	22	0
50	E	4	0	0	0	0
50	G	4	0	0	0	0
51	F	31	0	19	1	0
52	G	1	0	0	0	0
53	J	70	0	84	0	0
53	L	76	0	99	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	M	100	0	156	3	0
53	N	80	0	107	0	0
53	P	83	0	116	1	0
53	X	100	0	156	1	0
53	d	65	0	77	2	0
53	i	80	0	104	1	0
53	q	61	0	66	0	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	31	0	12	3	0
56	O	1	0	0	0	0
57	P	48	0	26	0	0
58	T	37	0	0	1	0
58	U	37	0	0	1	0
59	i	29	0	38	4	0
60	o	15	0	27	0	0
All	All	70020	0	71293	471	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (471) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:VAL:HG11	6:F:192:LEU:HD21	1.46	0.95
7:G:140:LYS:O	7:G:148:THR:OG1	1.90	0.88
32:g:25:ARG:O	32:g:25:ARG:NE	2.08	0.86
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.57	0.86
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.10	0.84
12:L:508:THR:O	39:n:35:LYS:NZ	2.10	0.84
11:K:97:GLN:OE1	12:L:587:TYR:OH	1.95	0.83
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.15	0.80
7:G:615:THR:OG1	7:G:617:ASP:OD1	2.01	0.79
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.02	0.77
1:A:71:LEU:O	10:J:147:TYR:OH	2.02	0.77
14:N:298:TYR:O	14:N:303:THR:OG1	2.02	0.77
10:J:77:GLU:N	10:J:77:GLU:OE1	2.18	0.76
12:L:161:ARG:NH1	12:L:238:GLU:OE1	2.17	0.76
24:Y:2:LYS:NZ	45:Y:205:3PE:O14	2.18	0.76
34:i:89:VAL:HG12	34:i:95:THR:HG21	1.69	0.74
45:J:203:3PE:O11	45:J:206:3PE:N	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:272:ASP:OD1	7:G:681:SER:OG	2.03	0.73
29:d:104:LYS:O	29:d:106:LYS:NZ	2.20	0.73
40:o:47:ASP:OD2	41:p:15:ARG:NH2	2.20	0.73
24:Y:13:GLU:OE2	24:Y:89:TYR:OH	2.06	0.73
35:j:29:SER:OG	36:k:68:LYS:O	2.06	0.72
12:L:561:ILE:O	12:L:565:THR:OG1	2.07	0.72
33:h:49:GLU:OE1	33:h:68:LYS:NZ	2.22	0.72
49:D:501:U10:C21	49:D:501:U10:H151	2.21	0.71
49:D:501:U10:H452	8:H:224:PHE:CD2	2.27	0.70
49:D:501:U10:H451	49:D:501:U10:C48	2.21	0.70
6:F:224:ASN:ND2	51:F:501:FMN:O2	2.25	0.70
34:i:89:VAL:HG12	34:i:95:THR:CG2	2.21	0.70
24:Y:16:GLU:OE1	24:Y:19:ARG:NE	2.26	0.69
14:N:215:MET:HE1	14:N:244:ILE:HG23	1.75	0.69
15:O:138:MET:HE3	55:O:401:DGT:HN2	1.57	0.68
12:L:245:ALA:O	12:L:249:SER:OG	2.11	0.68
2:B:76:PHE:CE2	49:D:501:U10:H152	2.29	0.68
7:G:644:GLN:N	7:G:644:GLN:OE1	2.27	0.67
12:L:161:ARG:NH2	39:n:87:GLY:O	2.27	0.67
33:h:62:GLU:OE1	33:h:64:TRP:NE1	2.27	0.67
6:F:257:ASN:ND2	6:F:267:THR:OG1	2.28	0.66
13:M:259:TYR:O	13:M:263:MET:HE2	1.95	0.66
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.28	0.66
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.78	0.66
3:C:183:VAL:O	22:W:100:THR:OG1	2.13	0.66
9:I:172:ASP:OD2	9:I:176:ARG:NH1	2.29	0.66
16:P:335:GLN:O	16:P:335:GLN:NE2	2.29	0.66
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.29	0.65
5:E:217:LEU:HD11	6:F:48:ILE:HG12	1.78	0.65
11:K:43:MET:SD	14:N:72:MET:HE1	2.36	0.65
7:G:415:LEU:O	7:G:416:THR:OG1	2.12	0.65
15:O:320:LYS:O	29:d:60:ARG:NH2	2.28	0.65
16:P:306:GLU:N	16:P:306:GLU:OE1	2.31	0.64
49:D:501:U10:H151	49:D:501:U10:H211	1.78	0.64
19:S:42:GLU:N	19:S:42:GLU:OE1	2.31	0.64
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.07	0.64
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.31	0.64
7:G:375:ASP:OD1	7:G:375:ASP:N	2.30	0.63
20:U:2:ASP:OD2	35:j:1:ALA:N	2.31	0.63
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	1.79	0.63
16:P:143:SER:OG	16:P:282:ASP:OD1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:141:GLU:N	37:l:141:GLU:OE1	2.31	0.63
15:O:281:GLU:N	15:O:281:GLU:OE1	2.31	0.63
6:F:367:GLU:OE2	7:G:135:ARG:NH2	2.32	0.63
23:X:87:CYS:SG	23:X:102:GLN:NE2	2.72	0.63
8:H:18:ALA:O	8:H:21:THR:OG1	2.16	0.63
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.24	0.63
11:K:59:MET:HE2	14:N:27:LEU:HD13	1.81	0.62
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.29	0.62
15:O:83:TYR:OH	55:O:401:DGT:O3'	2.07	0.62
6:F:194:GLU:OE2	17:Q:133:LYS:NZ	2.33	0.62
15:O:32:CYS:SG	15:O:186:LYS:NZ	2.71	0.62
40:o:91:HIS:O	40:o:95:VAL:HG23	1.99	0.62
42:q:78:ASP:OD1	42:q:80:SER:OG	2.18	0.62
15:O:173:ASP:OD2	15:O:207:LYS:NZ	2.19	0.62
23:X:102:GLN:N	23:X:102:GLN:OE1	2.33	0.62
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.82	0.61
59:i:201:CHD:H212	59:i:201:CHD:H12	1.82	0.61
13:M:141:GLU:N	13:M:141:GLU:OE1	2.33	0.61
16:P:268:ARG:NH2	47:P:505:PLC:O2P	2.34	0.61
7:G:339:ASP:OD1	19:S:16:ARG:NH1	2.34	0.61
15:O:82:PHE:CE1	15:O:138:MET:HE2	2.36	0.61
12:L:71:ILE:HG23	13:M:310:MET:HE1	1.83	0.61
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.36	0.61
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.81	0.61
12:L:194:ASN:ND2	41:p:106:GLN:OE1	2.33	0.61
18:R:1:GLY:N	18:R:42:ASP:OD2	2.30	0.61
29:d:3:THR:HG23	29:d:4:GLY:H	1.66	0.60
37:l:132:GLN:OE1	40:o:36:ARG:NH1	2.34	0.60
10:J:157:THR:HG22	11:K:66:PHE:HE1	1.66	0.60
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.83	0.60
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.83	0.60
45:L:705:3PE:N	45:Y:203:3PE:O12	2.32	0.60
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.83	0.60
1:A:1:FME:O1	1:A:2:ASN:N	2.34	0.60
16:P:13:ARG:NH2	16:P:61:PRO:O	2.34	0.60
39:n:133:GLU:N	39:n:133:GLU:OE1	2.35	0.60
8:H:249:PRO:O	26:a:28:ARG:NH2	2.35	0.59
11:K:59:MET:CE	14:N:27:LEU:HD13	2.32	0.59
35:j:69:ASP:OD2	40:o:113:ARG:NE	2.33	0.59
12:L:341:MET:CE	12:L:457:LEU:HD12	2.33	0.59
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:U:101:EHZ:O7	39:n:12:GLN:NE2	2.36	0.59
46:g:202:PC1:O13	46:g:202:PC1:H132	2.03	0.59
23:X:150:ASN:OD1	30:e:50:ARG:NH1	2.35	0.59
7:G:684:MET:HA	7:G:684:MET:HE2	1.85	0.58
2:B:69:MET:HE1	2:B:76:PHE:CD2	2.37	0.58
1:A:54:LYS:HG3	1:A:114:THR:HG23	1.85	0.58
23:X:11:ASP:O	23:X:60:LYS:NZ	2.25	0.58
23:X:44:LEU:HD22	23:X:130:VAL:HG13	1.85	0.58
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.37	0.58
44:s:58:LEU:O	44:s:62:ARG:NE	2.36	0.58
4:D:227:GLU:OE2	9:I:32:ARG:NH2	2.36	0.58
2:B:44:SER:O	8:H:54:LYS:NZ	2.36	0.58
10:J:23:LYS:NZ	11:K:21:MET:O	2.24	0.58
10:J:103:MET:HA	10:J:103:MET:HE2	1.85	0.58
49:D:501:U10:H151	49:D:501:U10:H212	1.85	0.58
7:G:53:ARG:O	7:G:93:VAL:HG21	2.02	0.58
4:D:343:GLU:N	4:D:343:GLU:OE1	2.37	0.58
29:d:112:VAL:O	41:p:159:LYS:NZ	2.37	0.58
3:C:83:ILE:HG22	3:C:85:THR:HG22	1.86	0.57
14:N:265:MET:HA	14:N:265:MET:HE2	1.85	0.57
14:N:7:ILE:HD13	47:O:403:PLC:H5'2	1.86	0.57
40:o:28:TYR:OH	40:o:110:ARG:NH1	2.37	0.57
18:R:55:ARG:NE	18:R:76:ASP:OD1	2.34	0.57
7:G:332:LYS:NZ	7:G:505:LEU:O	2.37	0.57
9:I:145:GLU:OE1	9:I:145:GLU:N	2.38	0.57
2:B:108:PRO:O	8:H:58:LYS:NZ	2.37	0.57
6:F:268:VAL:HG21	6:F:283:HIS:ND1	2.19	0.57
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.39	0.57
40:o:82:GLU:OE1	40:o:82:GLU:N	2.37	0.57
6:F:47:GLU:N	6:F:47:GLU:OE1	2.36	0.57
59:i:201:CHD:O3	59:i:201:CHD:H9	2.04	0.56
7:G:372:GLU:OE2	7:G:394:ARG:NH1	2.36	0.56
49:D:501:U10:H211	49:D:501:U10:H162	1.88	0.56
37:l:5:THR:OG1	37:l:7:ASP:OD1	2.14	0.56
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.88	0.56
37:l:65:ASP:OD1	38:m:43:LYS:NZ	2.37	0.56
17:Q:62:ARG:NH1	22:W:126:ASP:OD2	2.38	0.56
1:A:53:MET:HE1	10:J:69:GLY:HA3	1.86	0.56
7:G:366:THR:HB	7:G:450:MET:HE3	1.87	0.56
25:Z:126:LEU:HD13	30:e:82:ARG:HD3	1.87	0.56
6:F:94:VAL:CG1	6:F:192:LEU:HD21	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:217:LEU:HD11	6:F:48:ILE:CG1	2.36	0.55
49:D:501:U10:H401	49:D:501:U10:C43	2.37	0.55
12:L:87:MET:HA	12:L:87:MET:HE2	1.86	0.55
3:C:85:THR:HG21	21:V:115:ILE:CG1	2.37	0.54
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.89	0.54
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.42	0.54
32:g:79:TYR:OH	53:i:202:CDL:OA7	2.18	0.54
49:D:501:U10:H412	49:D:501:U10:H351	1.90	0.54
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.38	0.54
6:F:96:ASN:ND2	6:F:187:GLY:O	2.36	0.54
5:E:63:ILE:O	5:E:67:ASN:ND2	2.40	0.54
5:E:149:VAL:HG13	6:F:105:CYS:SG	2.47	0.54
13:M:208:PRO:HG3	13:M:216:LEU:HD13	1.90	0.54
13:M:271:MET:HE2	13:M:271:MET:HA	1.90	0.54
58:T:101:EHZ:O1	58:T:101:EHZ:O2	2.25	0.54
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.90	0.54
12:L:358:LYS:NZ	39:n:27:GLU:OE2	2.41	0.54
38:m:83:THR:OG1	45:m:201:3PE:O12	2.26	0.53
7:G:328:LEU:O	7:G:507:TYR:OH	2.23	0.53
16:P:5:VAL:HG12	16:P:5:VAL:O	2.09	0.53
49:D:501:U10:H4M3	49:D:501:U10:H3M2	1.88	0.53
14:N:72:MET:HE2	14:N:76:ILE:HG13	1.91	0.53
8:H:248:ASN:OD1	8:H:251:MET:N	2.41	0.53
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.91	0.53
10:J:81:GLU:OE1	11:K:23:ARG:NH1	2.40	0.53
10:J:167:VAL:HG13	14:N:42:PRO:HG3	1.89	0.53
13:M:304:GLN:O	29:d:119:VAL:HG11	2.08	0.53
20:U:23:ASP:OD1	36:k:46:ARG:NH2	2.41	0.53
32:g:101:GLU:HG3	32:g:107:ILE:HD11	1.91	0.52
13:M:127:VAL:HG11	53:M:602:CDL:H842	1.91	0.52
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.91	0.52
25:Z:27:ARG:NH2	43:r:13:TRP:O	2.41	0.52
23:X:90:TYR:OH	26:a:28:ARG:NH2	2.42	0.52
59:i:201:CHD:O7	59:i:201:CHD:H41	2.10	0.52
6:F:394:GLU:OE1	7:G:129:ARG:NH1	2.38	0.52
12:L:140:LEU:O	12:L:140:LEU:HD23	2.10	0.52
7:G:190:MET:HE1	7:G:690:ALA:HB1	1.92	0.52
7:G:675:ASP:OD1	7:G:678:SER:OG	2.15	0.52
3:C:154:ASP:OD1	3:C:155:TYR:N	2.43	0.52
7:G:281:GLU:OE1	7:G:293:HIS:ND1	2.43	0.52
13:M:113:MET:SD	13:M:175:ASN:ND2	2.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:M:602:CDL:O1	15:O:303:LYS:NZ	2.43	0.52
6:F:192:LEU:HD23	6:F:193:ILE:N	2.25	0.51
7:G:47:SER:OG	7:G:165:GLU:OE2	2.24	0.51
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.93	0.51
25:Z:104:LYS:O	30:e:74:ARG:NH2	2.43	0.51
49:D:501:U10:H452	8:H:224:PHE:CG	2.46	0.51
3:C:112:ASP:OD1	3:C:115:THR:OG1	2.24	0.51
4:D:347:HIS:CD2	7:G:121:MET:HE3	2.44	0.51
4:D:413:ASP:OD1	8:H:281:ARG:NH1	2.44	0.51
6:F:292:ASP:O	6:F:339:ARG:NH2	2.43	0.51
13:M:423:ILE:HD12	38:m:58:VAL:HG22	1.92	0.51
10:J:157:THR:HG22	11:K:66:PHE:CE1	2.46	0.51
19:S:94:LEU:O	19:S:97:LYS:NZ	2.39	0.51
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.15	0.50
2:B:92:LEU:HD13	2:B:100:LEU:HD13	1.93	0.50
13:M:255:ASP:OD2	45:M:603:3PE:N	2.39	0.50
29:d:3:THR:HG23	29:d:4:GLY:N	2.26	0.50
15:O:250:ASP:OD1	15:O:250:ASP:N	2.44	0.50
1:A:35:SER:O	2:B:81:ARG:NH2	2.45	0.50
4:D:152:MET:O	4:D:156:THR:OG1	2.22	0.50
13:M:165:ILE:HG21	14:N:268:GLN:HA	1.94	0.50
40:o:102:GLU:OE2	40:o:105:ARG:NH1	2.45	0.50
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.94	0.50
12:L:562:LEU:HB2	12:L:563:PRO:HD3	1.93	0.50
34:i:48:LYS:O	34:i:51:GLN:NE2	2.45	0.50
12:L:194:ASN:ND2	12:L:194:ASN:O	2.45	0.50
25:Z:126:LEU:HD22	30:e:82:ARG:HE	1.77	0.50
31:f:5:GLN:OE1	31:f:8:ARG:NH1	2.43	0.50
12:L:264:TYR:N	12:L:265:PRO:CD	2.76	0.49
5:E:105:THR:HG22	5:E:106:THR:H	1.76	0.49
2:B:69:MET:HE1	2:B:76:PHE:HD2	1.76	0.49
23:X:109:CYS:SG	23:X:110:VAL:N	2.86	0.49
4:D:282:GLU:N	4:D:282:GLU:OE1	2.45	0.49
12:L:489:THR:O	12:L:493:VAL:HG22	2.12	0.49
13:M:3:LYS:NZ	31:f:27:ASP:OD2	2.37	0.49
8:H:72:ILE:HD12	53:P:502:CDL:OA9	2.13	0.49
15:O:104:ARG:NE	15:O:131:ASP:OD1	2.44	0.49
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.94	0.49
49:D:501:U10:H502	8:H:221:ALA:HB1	1.95	0.49
5:E:55:GLN:O	5:E:59:GLY:N	2.41	0.49
12:L:398:ALA:O	12:L:402:SER:OG	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:31:ILE:O	15:O:179:VAL:HG13	2.12	0.48
18:R:78:GLU:OE1	18:R:96:HIS:ND1	2.46	0.48
4:D:128:ILE:HD13	4:D:330:VAL:HG11	1.95	0.48
6:F:93:LEU:HD13	6:F:129:MET:HE1	1.94	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.77	0.48
37:l:57:GLU:OE2	38:m:12:SER:OG	2.27	0.48
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.49	0.48
25:Z:85:MET:HE1	25:Z:124:TYR:CZ	2.48	0.48
4:D:335:ARG:NH2	9:I:126:CYS:O	2.37	0.48
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.44	0.48
6:F:370:ASP:OD2	6:F:374:LYS:NZ	2.46	0.48
9:I:76:ARG:O	9:I:128:VAL:HG21	2.13	0.48
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.48	0.48
4:D:167:PHE:CD2	49:D:501:U10:H202	2.48	0.48
7:G:192:MET:HE2	7:G:192:MET:HA	1.96	0.48
12:L:54:PHE:O	12:L:58:GLY:N	2.45	0.47
12:L:577:VAL:HG13	12:L:578:THR:HG23	1.95	0.47
14:N:146:PHE:N	14:N:147:PRO:CD	2.77	0.47
5:E:191:PHE:N	5:E:194:GLU:OE2	2.44	0.47
6:F:99:GLU:O	6:F:139:ARG:NE	2.47	0.47
9:I:144:HIS:O	9:I:144:HIS:ND1	2.43	0.47
13:M:187:HIS:O	13:M:192:ASN:ND2	2.40	0.47
37:l:32:GLU:N	37:l:32:GLU:OE1	2.46	0.47
53:M:602:CDL:H272	53:X:201:CDL:H671	1.96	0.47
3:C:58:ILE:HD11	3:C:119:SER:O	2.15	0.47
22:W:88:GLU:OE1	22:W:97:LYS:NZ	2.27	0.47
34:i:35:PRO:O	34:i:37:GLN:NE2	2.47	0.47
46:I:203:PC1:O13	46:I:203:PC1:H132	2.14	0.47
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.96	0.47
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.49	0.47
31:f:18:MET:HE3	31:f:18:MET:HA	1.96	0.47
33:h:52:LEU:C	33:h:52:LEU:HD13	2.40	0.47
43:r:72:GLN:N	43:r:72:GLN:OE1	2.48	0.47
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.95	0.47
3:C:8:ARG:O	4:D:129:ARG:NH2	2.42	0.47
8:H:317:GLN:OE1	10:J:141:MET:HE1	2.15	0.47
17:Q:89:LYS:HD2	17:Q:105:VAL:HG11	1.97	0.47
22:W:51:LEU:HD11	22:W:102:VAL:HG11	1.96	0.47
37:l:88:ARG:O	37:l:89:VAL:C	2.58	0.47
2:B:50:PHE:CE2	2:B:100:LEU:HD12	2.50	0.47
4:D:167:PHE:CE2	49:D:501:U10:H202	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.47	0.47
4:D:352:TYR:HD1	9:I:86:VAL:HG21	1.80	0.46
31:f:53:GLU:N	31:f:53:GLU:OE1	2.48	0.46
4:D:135:GLN:HB3	4:D:277:VAL:HG13	1.97	0.46
7:G:24:THR:O	7:G:73:VAL:HG23	2.15	0.46
10:J:170:GLU:OE1	10:J:173:ARG:NH1	2.46	0.46
2:B:61:HIS:ND1	4:D:175:GLU:OE1	2.45	0.46
39:n:56:MET:HA	39:n:56:MET:HE2	1.98	0.46
6:F:192:LEU:HD23	6:F:192:LEU:C	2.40	0.46
15:O:260:ARG:HA	15:O:263:VAL:HG22	1.97	0.46
26:a:49:GLU:OE1	26:a:52:ARG:NH2	2.45	0.46
39:n:14:LYS:HB3	39:n:63:LEU:HD21	1.97	0.46
42:q:138:VAL:HG23	42:q:138:VAL:O	2.15	0.46
12:L:183:ILE:HD12	13:M:400:MET:HE1	1.96	0.46
13:M:130:LEU:HD21	14:N:294:MET:CE	2.46	0.46
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.50	0.46
4:D:238:ARG:NH1	8:H:279:ARG:O	2.41	0.46
6:F:327:THR:OG1	6:F:328:GLY:N	2.48	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.78	0.46
49:D:501:U10:H401	49:D:501:U10:H43	1.96	0.46
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.98	0.46
11:K:37:MET:SD	14:N:68:MET:HE1	2.55	0.46
7:G:366:THR:HG22	7:G:366:THR:O	2.16	0.46
12:L:76:LEU:HD21	12:L:196:TRP:HE3	1.81	0.46
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.97	0.46
34:i:125:GLN:O	34:i:126:HIS:ND1	2.49	0.46
44:s:42:GLN:OE1	44:s:42:GLN:N	2.44	0.45
7:G:533:THR:HG23	7:G:535:GLN:H	1.82	0.45
20:U:49:GLU:OE2	39:n:19:TYR:OH	2.34	0.45
23:X:58:GLU:OE1	23:X:58:GLU:N	2.43	0.45
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.98	0.45
8:H:285:LEU:HD12	8:H:289:LEU:HD13	1.99	0.45
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.97	0.45
49:D:501:U10:H503	8:H:52:ALA:HA	1.98	0.45
12:L:133:THR:HG22	12:L:133:THR:O	2.15	0.45
46:L:706:PC1:H142	46:L:706:PC1:O13	2.17	0.45
30:e:45:GLY:O	33:h:124:HIS:NE2	2.45	0.45
7:G:143:GLY:HA2	7:G:190:MET:HE2	1.99	0.45
11:K:43:MET:CE	14:N:72:MET:HE1	2.47	0.45
14:N:72:MET:HA	14:N:72:MET:HE3	1.99	0.45
16:P:203:GLN:NE2	16:P:232:GLY:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:VAL:HG21	6:F:122:CYS:SG	2.57	0.45
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.52	0.45
16:P:271:GLU:HG2	16:P:280:THR:HG22	1.98	0.45
4:D:165:THR:HG21	8:H:275:ALA:O	2.16	0.45
29:d:60:ARG:NH1	53:d:201:CDL:OA3	2.49	0.45
41:p:5:ASP:OD1	41:p:7:ASP:N	2.47	0.45
6:F:30:ASP:OD1	6:F:32:ARG:NH1	2.49	0.45
6:F:188:GLU:OE1	6:F:190:THR:OG1	2.27	0.45
42:q:143:PRO:O	42:q:144:TYR:CD2	2.71	0.45
44:s:31:GLU:N	44:s:32:PRO:CD	2.80	0.45
6:F:306:LEU:C	6:F:306:LEU:HD12	2.42	0.44
12:L:598:SER:CB	14:N:100:MET:HE1	2.47	0.44
1:A:73:LEU:N	1:A:74:PRO:CD	2.80	0.44
12:L:581:LYS:CD	12:L:586:LEU:HD12	2.47	0.44
12:L:603:ASN:ND2	12:L:606:GLU:OE1	2.50	0.44
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.48	0.44
13:M:207:MET:O	13:M:208:PRO:C	2.61	0.44
24:Y:81:GLU:OE1	24:Y:81:GLU:N	2.51	0.44
3:C:33:LEU:HD23	21:V:98:PRO:HB2	2.00	0.44
6:F:234:ILE:O	6:F:238:GLY:N	2.50	0.44
12:L:581:LYS:HZ3	12:L:586:LEU:HD12	1.82	0.44
26:a:43:TYR:CZ	26:a:47:LEU:HD11	2.52	0.44
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.53	0.44
39:n:177:PRO:O	39:n:178:MET:C	2.60	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.44
37:l:82:ASP:OD1	37:l:82:ASP:N	2.50	0.44
2:B:45:LEU:HD22	2:B:85:VAL:CG2	2.48	0.44
4:D:159:LEU:CD2	49:D:501:U10:H203	2.48	0.44
12:L:173:LEU:C	12:L:173:LEU:HD23	2.43	0.44
12:L:195:THR:HG21	12:L:200:GLN:HB3	2.00	0.44
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.17	0.44
49:D:501:U10:H362	49:D:501:U10:H312	2.00	0.43
6:F:258:ILE:N	6:F:258:ILE:HD12	2.33	0.43
7:G:315:VAL:O	7:G:340:SER:OG	2.33	0.43
12:L:383:MET:HB3	12:L:386:LEU:HD12	2.00	0.43
29:d:5:ARG:CZ	29:d:85:VAL:HG13	2.48	0.43
2:B:91:THR:HA	2:B:119:CYS:HB3	2.00	0.43
49:D:501:U10:H352	8:H:25:ARG:HG3	1.99	0.43
5:E:181:ILE:N	5:E:181:ILE:HD12	2.32	0.43
10:J:167:VAL:HG22	14:N:42:PRO:HG2	1.99	0.43
12:L:323:TYR:CZ	12:L:475:THR:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:48:ASP:OD1	32:g:49:LYS:N	2.50	0.43
7:G:371:VAL:HG22	7:G:450:MET:HE1	2.00	0.43
13:M:208:PRO:HD3	13:M:236:LEU:HD22	2.00	0.43
16:P:46:ILE:N	16:P:46:ILE:HD12	2.33	0.43
25:Z:85:MET:HE1	25:Z:124:TYR:CE2	2.53	0.43
29:d:71:VAL:HG11	53:d:201:CDL:H431	2.01	0.43
2:B:75:VAL:HG11	49:D:501:U10:C38	2.48	0.43
47:A:206:PLC:H12	27:b:38:THR:HG21	2.01	0.43
2:B:81:ARG:HA	2:B:108:PRO:HD3	2.00	0.43
5:E:190:ARG:NE	5:E:192:SER:O	2.52	0.43
8:H:49:ILE:N	8:H:49:ILE:HD12	2.34	0.43
12:L:278:LEU:HD21	12:L:404:THR:OG1	2.19	0.43
20:T:32:VAL:O	20:T:32:VAL:HG12	2.18	0.43
33:h:140:THR:O	33:h:143:ASN:ND2	2.48	0.43
44:s:63:MET:HE2	44:s:64:PRO:HD2	2.00	0.43
4:D:279:ASP:OD1	4:D:279:ASP:N	2.51	0.43
37:l:80:ASP:HB3	37:l:83:MET:HE2	2.00	0.43
42:q:2:GLU:OE2	43:r:5:ARG:N	2.38	0.43
1:A:67:LEU:HD13	11:K:65:VAL:HA	2.00	0.43
46:A:202:PC1:H321	8:H:72:ILE:HG21	1.99	0.43
3:C:8:ARG:NH1	43:r:61:GLU:OE2	2.39	0.43
6:F:49:LEU:HD22	6:F:127:ARG:HG3	2.00	0.43
12:L:183:ILE:HG21	13:M:382:VAL:HG11	2.00	0.43
14:N:342:MET:O	14:N:345:VAL:HG22	2.19	0.43
42:q:5:GLN:N	42:q:5:GLN:OE1	2.52	0.43
13:M:108:MET:CB	13:M:121:LEU:HD13	2.48	0.43
13:M:373:ILE:HD11	13:M:444:LEU:HD12	2.01	0.43
14:N:182:SER:OG	14:N:293:TYR:OH	2.16	0.43
16:P:26:ALA:HB3	16:P:47:VAL:HG13	2.01	0.43
59:i:201:CHD:H183	59:i:201:CHD:H20	1.79	0.43
4:D:165:THR:N	4:D:166:PRO:CD	2.82	0.43
39:n:30:CYS:O	39:n:32:HIS:N	2.52	0.43
8:H:28:LEU:HD22	8:H:275:ALA:HB2	2.01	0.42
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.43	0.42
34:i:89:VAL:HG12	34:i:95:THR:HG23	1.98	0.42
35:j:7:ILE:HG23	35:j:16:GLN:HB3	2.00	0.42
3:C:85:THR:HG21	21:V:115:ILE:HG13	2.00	0.42
4:D:218:PHE:CE2	4:D:222:ILE:HD11	2.54	0.42
8:H:301:CYS:O	8:H:305:VAL:HG23	2.19	0.42
14:N:261:MET:HG3	14:N:340:THR:HG23	2.00	0.42
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:94:THR:OG1	37:l:96:VAL:O	2.32	0.42
7:G:113:GLU:OE2	7:G:249:ARG:NH2	2.51	0.42
38:m:22:TYR:C	38:m:24:ILE:HD13	2.45	0.42
4:D:81:GLY:N	4:D:429:ASP:OD1	2.52	0.42
5:E:165:THR:HG23	5:E:167:LYS:H	1.83	0.42
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.84	0.42
14:N:331:VAL:HG13	14:N:335:MET:HE3	2.02	0.42
24:Y:74:CYS:SG	24:Y:75:ILE:N	2.92	0.42
27:b:47:ALA:HB1	27:b:77:LEU:HD21	2.01	0.42
27:b:61:ASN:ND2	27:b:61:ASN:O	2.52	0.42
13:M:204:MET:O	13:M:207:MET:O	2.37	0.42
20:U:87:TYR:OH	34:i:26:GLU:OE2	2.28	0.42
10:J:23:LYS:NZ	11:K:18:GLY:O	2.53	0.42
1:A:73:LEU:O	1:A:76:PRO:HD2	2.19	0.42
49:D:501:U10:H312	49:D:501:U10:C36	2.50	0.42
12:L:598:SER:HB2	14:N:100:MET:HE1	2.01	0.42
13:M:285:LEU:HD23	13:M:285:LEU:C	2.45	0.42
14:N:343:LEU:C	14:N:343:LEU:HD12	2.44	0.42
15:O:30:ASN:OD1	15:O:31:ILE:N	2.44	0.42
32:g:113:PHE:CE1	41:p:73:ILE:HG22	2.55	0.42
2:B:42:ARG:NH1	46:B:203:PC1:O14	2.40	0.42
6:F:362:CYS:HA	7:G:51:ASN:O	2.19	0.42
37:l:4:ILE:N	37:l:4:ILE:HD12	2.35	0.42
7:G:551:ASP:OD2	7:G:679:ARG:NH2	2.47	0.42
10:J:123:GLY:O	10:J:126:VAL:HG22	2.19	0.42
10:J:141:MET:HE3	30:e:26:HIS:CE1	2.55	0.42
32:g:64:PHE:O	32:g:69:VAL:HG23	2.20	0.42
32:g:98:LYS:NZ	41:p:5:ASP:OD2	2.48	0.42
37:l:141:GLU:OE2	40:o:42:GLN:NE2	2.52	0.42
2:B:49:THR:CG2	49:D:501:U10:H101	2.50	0.42
12:L:131:LEU:HD23	12:L:131:LEU:C	2.44	0.42
13:M:22:MET:HE3	32:g:53:VAL:HG13	2.02	0.42
24:Y:120:THR:O	24:Y:124:VAL:HG23	2.19	0.42
12:L:260:LEU:HD12	12:L:314:MET:HE2	2.02	0.41
8:H:307:LEU:HD21	25:Z:46:TYR:CD1	2.56	0.41
15:O:56:ILE:N	15:O:56:ILE:HD12	2.35	0.41
5:E:18:GLU:N	5:E:18:GLU:OE1	2.54	0.41
13:M:130:LEU:HD21	14:N:294:MET:HE2	2.02	0.41
13:M:457:PRO:O	32:g:84:ARG:NH1	2.43	0.41
7:G:627:SER:OG	7:G:629:ASN:OD1	2.38	0.41
11:K:96:LEU:O	11:K:98:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:22:LEU:HD23	19:S:22:LEU:N	2.35	0.41
39:n:50:HIS:CD2	39:n:62:LEU:HD13	2.55	0.41
40:o:88:TYR:CE2	40:o:92:LEU:HD11	2.56	0.41
5:E:16:ASN:HB2	5:E:17:PRO:HD2	2.03	0.41
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.02	0.41
15:O:35:LYS:NZ	55:O:401:DGT:O1A	2.54	0.41
23:X:138:GLU:N	23:X:138:GLU:OE1	2.53	0.41
26:a:6:LEU:HB3	45:a:101:3PE:H3I1	2.03	0.41
6:F:141:GLU:OE1	6:F:141:GLU:N	2.45	0.41
9:I:132:VAL:HG21	9:I:165:ILE:HG21	2.02	0.41
17:Q:10:LEU:N	17:Q:10:LEU:HD12	2.35	0.41
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.02	0.41
24:Y:100:LEU:O	24:Y:104:THR:HG22	2.20	0.41
24:Y:125:LYS:NZ	24:Y:129:LEU:HD21	2.36	0.41
25:Z:126:LEU:HD13	30:e:82:ARG:CD	2.50	0.41
25:Z:126:LEU:HD22	30:e:82:ARG:NE	2.36	0.41
10:J:5:ILE:HG23	10:J:6:VAL:N	2.35	0.41
1:A:115:GLU:N	1:A:115:GLU:OE1	2.54	0.41
2:B:96:MET:SD	4:D:82:LEU:HD23	2.61	0.41
4:D:371:LYS:NZ	4:D:424:VAL:HG23	2.36	0.41
7:G:326:GLU:OE1	7:G:326:GLU:N	2.48	0.41
46:H:401:PC1:O13	46:H:401:PC1:H133	2.21	0.41
13:M:133:ILE:HD11	13:M:231:LEU:HD11	2.01	0.41
13:M:423:ILE:CD1	38:m:58:VAL:HG13	2.51	0.41
23:X:79:GLU:HB3	23:X:80:PRO:HD3	2.03	0.41
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.02	0.41
14:N:68:MET:HA	14:N:68:MET:HE2	2.02	0.41
6:F:407:LEU:C	6:F:407:LEU:HD23	2.45	0.40
9:I:50:TYR:CG	9:I:51:PRO:HA	2.56	0.40
16:P:322:ARG:NH2	16:P:329:SER:O	2.51	0.40
20:T:6:LEU:HB3	20:T:86:VAL:HG21	2.03	0.40
29:d:105:ASP:OD1	29:d:105:ASP:N	2.53	0.40
4:D:350:LYS:HB2	7:G:121:MET:SD	2.61	0.40
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.02	0.40
21:V:8:THR:HG23	21:V:15:VAL:HG22	2.03	0.40
36:k:60:VAL:HG12	36:k:61:SER:N	2.37	0.40
20:T:36:PHE:HD1	20:T:40:LEU:HD12	1.87	0.40
6:F:258:ILE:HG21	6:F:284:ALA:CB	2.52	0.40
6:F:342:ASP:OD1	6:F:429:ARG:NH2	2.51	0.40
7:G:185:THR:O	7:G:187:ILE:N	2.51	0.40
25:Z:88:GLU:OE1	25:Z:127:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:PRO:HB3	48:B:201:SF4:S1	2.62	0.40
9:I:79:ALA:HB2	9:I:106:THR:HG23	2.02	0.40
10:J:1:FME:SD	10:J:2:MET:N	2.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
2	B	153/216 (71%)	148 (97%)	5 (3%)	0	100	100
3	C	207/266 (78%)	204 (99%)	3 (1%)	0	100	100
4	D	427/463 (92%)	414 (97%)	13 (3%)	0	100	100
5	E	212/249 (85%)	204 (96%)	8 (4%)	0	100	100
6	F	430/464 (93%)	424 (99%)	6 (1%)	0	100	100
7	G	691/727 (95%)	672 (97%)	19 (3%)	0	100	100
8	H	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
11	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
12	L	604/606 (100%)	581 (96%)	23 (4%)	0	100	100
13	M	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	340/380 (90%)	330 (97%)	10 (3%)	0	100	100
17	Q	127/175 (73%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	94/124 (76%)	91 (97%)	3 (3%)	0	100	100
19	S	85/99 (86%)	84 (99%)	1 (1%)	0	100	100
20	T	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
20	U	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
21	V	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
22	W	113/128 (88%)	111 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
30	e	97/106 (92%)	96 (99%)	1 (1%)	0	100	100
31	f	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
32	g	99/154 (64%)	92 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	69 (100%)	0	0	100	100
36	k	79/98 (81%)	77 (98%)	2 (2%)	0	100	100
37	l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
38	m	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
41	p	172/176 (98%)	168 (98%)	4 (2%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	91/113 (80%)	89 (98%)	2 (2%)	0	100	100
44	s	43/109 (39%)	42 (98%)	1 (2%)	0	100	100
All	All	8198/9213 (89%)	7984 (97%)	214 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	97 (97%)	3 (3%)	36	66
2	B	131/175 (75%)	127 (97%)	4 (3%)	35	65
3	C	190/228 (83%)	188 (99%)	2 (1%)	65	85
4	D	370/392 (94%)	368 (100%)	2 (0%)	81	92
5	E	183/205 (89%)	176 (96%)	7 (4%)	29	58
6	F	346/368 (94%)	334 (96%)	12 (4%)	32	61
7	G	583/608 (96%)	569 (98%)	14 (2%)	43	72
8	H	274/274 (100%)	272 (99%)	2 (1%)	76	90
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	83
10	J	141/141 (100%)	138 (98%)	3 (2%)	47	75
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	72
12	L	533/533 (100%)	524 (98%)	9 (2%)	53	79
13	M	412/412 (100%)	404 (98%)	8 (2%)	50	77
14	N	315/315 (100%)	312 (99%)	3 (1%)	68	86
15	O	283/303 (93%)	275 (97%)	8 (3%)	38	68
16	P	296/327 (90%)	281 (95%)	15 (5%)	21	48
17	Q	116/153 (76%)	110 (95%)	6 (5%)	21	47
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	83
19	S	77/82 (94%)	74 (96%)	3 (4%)	28	57
20	T	81/135 (60%)	73 (90%)	8 (10%)	7	19
20	U	81/135 (60%)	76 (94%)	5 (6%)	16	39
21	V	101/102 (99%)	99 (98%)	2 (2%)	48	76
22	W	107/114 (94%)	106 (99%)	1 (1%)	70	87
23	X	154/155 (99%)	150 (97%)	4 (3%)	40	70
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	115 (96%)	5 (4%)	26	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	43 (96%)	2 (4%)	25	53
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	67
30	e	89/96 (93%)	86 (97%)	3 (3%)	32	62
31	f	54/54 (100%)	52 (96%)	2 (4%)	30	59
32	g	92/131 (70%)	89 (97%)	3 (3%)	33	63
33	h	121/158 (77%)	117 (97%)	4 (3%)	33	63
34	i	120/121 (99%)	115 (96%)	5 (4%)	26	55
35	j	61/84 (73%)	57 (93%)	4 (7%)	15	36
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	80
37	l	140/159 (88%)	136 (97%)	4 (3%)	37	67
38	m	113/114 (99%)	108 (96%)	5 (4%)	25	53
39	n	156/161 (97%)	151 (97%)	5 (3%)	34	64
40	o	110/120 (92%)	103 (94%)	7 (6%)	16	38
41	p	155/157 (99%)	150 (97%)	5 (3%)	34	64
42	q	130/130 (100%)	125 (96%)	5 (4%)	29	58
43	r	85/97 (88%)	84 (99%)	1 (1%)	63	84
44	s	44/92 (48%)	44 (100%)	0	100	100
All	All	7223/7891 (92%)	7033 (97%)	190 (3%)	41	70

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	MET
1	A	68	GLU
1	A	109	LYS
2	B	54	CYS
2	B	69	MET
2	B	84	ASP
2	B	171	LYS
3	C	20	LYS
3	C	125	LYS
4	D	40	LYS
4	D	411	LEU

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Mol	Chain	Res	Type
5	E	68	LYS
5	E	72	ILE
5	E	148	CYS
5	E	165	THR
5	E	183	LYS
5	E	190	ARG
5	E	194	GLU
6	F	8	LYS
6	F	16	LYS
6	F	32	ARG
6	F	46	LYS
6	F	84	LYS
6	F	105	CYS
6	F	127	ARG
6	F	132	ARG
6	F	192	LEU
6	F	248	GLU
6	F	359	CYS
6	F	365	CYS
7	G	73	VAL
7	G	85	LYS
7	G	122	MET
7	G	135	ARG
7	G	177	ARG
7	G	192	MET
7	G	229	ASP
7	G	249	ARG
7	G	287	GLU
7	G	375	ASP
7	G	408	LEU
7	G	516	LYS
7	G	669	LYS
7	G	704	CYS
8	H	14	LEU
8	H	70	MET
9	I	54	LYS
9	I	176	ARG
10	J	87	LYS
10	J	139	GLU
10	J	141	MET
11	K	59	MET
11	K	95	LEU

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Mol	Chain	Res	Type
12	L	88	MET
12	L	336	LYS
12	L	364	LYS
12	L	479	GLN
12	L	481	THR
12	L	487	LYS
12	L	512	LYS
12	L	581	LYS
12	L	583	LEU
13	M	19	LYS
13	M	22	MET
13	M	72	LEU
13	M	91	ARG
13	M	116	ILE
13	M	123	GLU
13	M	138	ASN
13	M	315	LEU
14	N	88	LYS
14	N	204	ASN
14	N	319	LEU
15	O	23	LYS
15	O	40	LYS
15	O	80	GLU
15	O	146	LYS
15	O	206	TYR
15	O	213	GLU
15	O	303	LYS
15	O	315	LYS
16	P	1	LEU
16	P	2	HIS
16	P	13	ARG
16	P	97	ARG
16	P	102	GLN
16	P	107	GLU
16	P	109	VAL
16	P	122	LYS
16	P	140	LYS
16	P	149	LYS
16	P	226	LYS
16	P	268	ARG
16	P	313	LYS
16	P	316	GLU

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Mol	Chain	Res	Type
16	P	335	GLN
17	Q	16	LYS
17	Q	42	ARG
17	Q	44	ASN
17	Q	70	MET
17	Q	116	LYS
17	Q	122	PHE
18	R	25	LYS
19	S	38	LYS
19	S	43	LEU
19	S	61	GLN
20	T	7	THR
20	T	12	LYS
20	T	20	LYS
20	T	29	LYS
20	T	38	LYS
20	T	71	MET
20	T	72	CYS
20	T	75	GLU
20	U	12	LYS
20	U	20	LYS
20	U	51	ILE
20	U	71	MET
20	U	83	LYS
21	V	65	LYS
21	V	115	ILE
22	W	86	LYS
23	X	11	ASP
23	X	15	GLN
23	X	16	GLU
23	X	57	GLU
25	Z	4	LYS
25	Z	50	MET
25	Z	51	LYS
25	Z	54	ARG
25	Z	98	LYS
28	c	1	LYS
28	c	16	LYS
29	d	25	LYS
29	d	106	LYS
29	d	120	ARG
30	e	7	LYS

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Mol	Chain	Res	Type
30	e	17	MET
30	e	91	TYR
31	f	18	MET
31	f	29	LYS
32	g	24	LEU
32	g	90	ARG
32	g	117	LYS
33	h	6	LYS
33	h	23	LYS
33	h	113	LEU
33	h	130	LYS
34	i	12	GLN
34	i	51	GLN
34	i	55	LEU
34	i	95	THR
34	i	98	GLU
35	j	39	ARG
35	j	40	PHE
35	j	47	VAL
35	j	50	HIS
36	k	91	LYS
37	l	4	ILE
37	l	6	LYS
37	l	25	LYS
37	l	126	GLN
38	m	24	ILE
38	m	29	ARG
38	m	49	GLN
38	m	79	PHE
38	m	119	LYS
39	n	14	LYS
39	n	56	MET
39	n	111	LYS
39	n	135	GLU
39	n	137	LYS
40	o	7	ARG
40	o	15	GLU
40	o	21	MET
40	o	47	ASP
40	o	83	ARG
40	o	105	ARG
40	o	111	LYS

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Mol	Chain	Res	Type
41	p	37	ASP
41	p	42	ARG
41	p	69	ARG
41	p	88	GLU
41	p	126	LYS
42	q	67	GLU
42	q	96	ASP
42	q	107	LYS
42	q	122	GLN
42	q	144	TYR
43	r	107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
3	C	19	HIS
3	C	39	GLN
3	C	46	ASN
3	C	88	ASN
3	C	160	HIS
3	C	192	GLN
4	D	217	ASN
5	E	150	ASN
5	E	157	ASN
6	F	257	ASN
7	G	179	ASN
7	G	402	ASN
7	G	459	GLN
7	G	515	GLN
8	H	47	GLN
8	H	99	ASN
11	K	50	ASN
12	L	31	ASN
12	L	56	HIS
12	L	72	GLN
12	L	135	ASN
12	L	194	ASN
12	L	603	ASN
13	M	138	ASN
13	M	366	ASN
18	R	90	GLN

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Mol	Chain	Res	Type
19	S	61	GLN
22	W	47	HIS
22	W	69	ASN
25	Z	60	GLN
26	a	27	HIS
27	b	51	ASN
27	b	61	ASN
27	b	70	GLN
29	d	61	GLN
30	e	26	HIS
30	e	81	GLN
31	f	51	ASN
33	h	135	HIS
37	l	66	HIS
39	n	52	ASN
40	o	75	ASN
40	o	91	HIS
41	p	27	ASN
41	p	106	GLN
41	p	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

15 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	FME	K	1	11	8,9,10	1.52	1 (12%)	8,9,11	1.36	1 (12%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	8,9,11	1.39	1 (12%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	8,9,11	1.33	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.27	1 (11%)
8	FME	H	1	8	8,9,10	1.52	1 (12%)	8,9,11	1.51	2 (25%)
4	2MR	D	85	4	10,12,13	2.50	2 (20%)	5,13,15	1.34	1 (20%)
34	SAC	i	1	34	7,8,9	1.74	1 (14%)	7,9,11	1.50	1 (14%)
1	FME	A	1	1	8,9,10	1.52	1 (12%)	8,9,11	1.29	1 (12%)
43	AYA	r	1	43	6,7,8	1.88	2 (33%)	6,8,10	1.29	1 (16%)
38	SAC	m	1	38	7,8,9	1.73	1 (14%)	7,9,11	1.31	1 (14%)
42	AME	q	1	42	9,10,11	1.55	1 (11%)	9,11,13	1.22	1 (11%)
13	FME	M	1	13	8,9,10	1.52	1 (12%)	8,9,11	1.42	1 (12%)
27	AYA	b	1	27	6,7,8	1.88	1 (16%)	6,8,10	1.44	1 (16%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	8,9,11	1.40	1 (12%)
24	AYA	Y	1	24	6,7,8	1.87	2 (33%)	6,8,10	1.31	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	K	1	11	-	3/7/9/11	-
14	FME	N	1	14	-	4/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-
29	AME	d	1	29	-	4/9/10/12	-
8	FME	H	1	8	-	4/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
34	SAC	i	1	34	-	2/7/8/10	-
1	FME	A	1	1	-	1/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
38	SAC	m	1	38	-	3/7/8/10	-
42	AME	q	1	42	-	3/9/10/12	-
13	FME	M	1	13	-	3/7/9/11	-
27	AYA	b	1	27	-	0/5/6/8	-
10	FME	J	1	10	-	4/7/9/11	-
24	AYA	Y	1	24	-	1/5/6/8	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.61	1.45	1.33
4	D	85	2MR	CZ-NE	5.19	1.45	1.34
1	A	1	FME	CN-N	3.78	1.45	1.33
11	K	1	FME	CN-N	3.77	1.45	1.33
13	M	1	FME	CN-N	3.76	1.45	1.33
10	J	1	FME	CN-N	3.76	1.45	1.33
12	L	1	FME	CN-N	3.75	1.45	1.33
8	H	1	FME	CN-N	3.74	1.45	1.33
14	N	1	FME	CN-N	3.73	1.45	1.33
42	q	1	AME	CT1-N	3.60	1.46	1.34
34	i	1	SAC	C1A-N	3.56	1.45	1.34
38	m	1	SAC	C1A-N	3.52	1.45	1.34
27	b	1	AYA	CT-N	3.49	1.45	1.34
24	Y	1	AYA	CT-N	3.46	1.45	1.34
43	r	1	AYA	CT-N	3.45	1.45	1.34
29	d	1	AME	CT1-N	3.44	1.45	1.34
43	r	1	AYA	OT-CT	-2.04	1.18	1.23
24	Y	1	AYA	OT-CT	-2.00	1.18	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	2.88	120.89	116.12
27	b	1	AYA	CM-CT-N	2.50	120.27	116.12
38	m	1	SAC	C2A-C1A-N	2.40	120.10	116.12
4	D	85	2MR	CD-NE-CZ	-2.37	118.92	123.36
8	H	1	FME	CE-SD-CG	2.33	112.36	100.32
24	Y	1	AYA	CM-CT-N	2.28	119.90	116.12
43	r	1	AYA	CM-CT-N	2.26	119.87	116.12
42	q	1	AME	CT2-CT1-N	2.15	119.69	116.12
14	N	1	FME	O1-CN-N	-2.14	119.80	125.32
29	d	1	AME	CT2-CT1-N	2.11	119.61	116.12
10	J	1	FME	O1-CN-N	-2.10	119.89	125.32
8	H	1	FME	O1-CN-N	-2.09	119.91	125.32
13	M	1	FME	O1-CN-N	-2.08	119.95	125.32
12	L	1	FME	O1-CN-N	-2.02	120.10	125.32
11	K	1	FME	O1-CN-N	-2.01	120.12	125.32
1	A	1	FME	O1-CN-N	-2.00	120.14	125.32

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	N-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	CB-CA-N-CN
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	CB-CA-N-CN
24	Y	1	AYA	O-C-CA-CB
29	d	1	AME	C-CA-CB-CG
29	d	1	AME	N-CA-CB-CG
42	q	1	AME	CB-CA-N-CT1
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
8	H	1	FME	CB-CG-SD-CE
12	L	1	FME	CA-CB-CG-SD
14	N	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CG-SD-CE
29	d	1	AME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
8	H	1	FME	CA-CB-CG-SD
38	m	1	SAC	C-CA-CB-OG
13	M	1	FME	N-CA-CB-CG
42	q	1	AME	CB-CG-SD-CE
38	m	1	SAC	CB-CA-N-C1A
11	K	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
38	m	1	SAC	C-CA-N-C1A
42	q	1	AME	C-CA-N-CT1
29	d	1	AME	CB-CA-N-CT1
8	H	1	FME	C-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
10	J	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 4 are monoatomic - leaving 82 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	I	204	-	43,43,53	1.05	4 (9%)	49,51,61	0.99	2 (4%)
46	PC1	J	202	-	34,34,53	1.18	4 (11%)	40,42,61	1.04	2 (5%)
48	SF4	G	802	7	0,12,12	-	-	-		
45	3PE	g	201	-	39,39,50	0.98	4 (10%)	42,44,55	1.10	2 (4%)
47	PLC	Y	207	-	35,35,41	0.55	0	41,43,49	0.52	0
47	PLC	B	202	-	36,36,41	0.54	0	42,44,49	0.52	0
46	PC1	I	203	-	53,53,53	0.94	4 (7%)	59,61,61	0.98	2 (3%)
46	PC1	H	401	-	47,47,53	1.01	4 (8%)	53,55,61	1.06	2 (3%)
48	SF4	I	202	9	0,12,12	-	-	-		
45	3PE	M	603	-	49,49,50	0.88	4 (8%)	52,54,55	1.04	2 (3%)
45	3PE	Y	205	-	38,38,50	0.99	4 (10%)	41,43,55	1.13	2 (4%)
45	3PE	A	204	-	30,30,50	1.11	4 (13%)	33,35,55	1.12	2 (6%)
45	3PE	p	201	-	34,34,50	0.98	3 (8%)	37,39,55	1.11	1 (2%)
45	3PE	Y	202	-	22,22,50	1.29	4 (18%)	25,27,55	1.25	2 (8%)
45	3PE	d	202	-	48,48,50	0.89	4 (8%)	51,53,55	1.06	2 (3%)
47	PLC	J	205	-	37,37,41	0.54	0	43,45,49	0.53	0
60	MYR	o	201	40	13,14,15	0.43	0	12,13,15	0.82	0
45	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.10	2 (4%)
45	3PE	Y	204	-	50,50,50	0.88	4 (8%)	53,55,55	1.02	2 (3%)
45	3PE	J	203	-	30,30,50	1.11	4 (13%)	33,35,55	1.15	2 (6%)
57	NDP	P	501	-	51,52,52	4.02	27 (52%)	71,80,80	1.90	15 (21%)
46	PC1	L	706	-	44,44,53	1.04	4 (9%)	50,52,61	1.04	2 (4%)
53	CDL	M	602	-	99,99,99	0.89	8 (8%)	105,111,111	1.13	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	L	705	-	50,50,50	0.87	4 (8%)	53,55,55	1.08	2 (3%)
47	PLC	O	403	-	31,31,41	0.57	0	37,39,49	0.60	0
45	3PE	I	205	-	37,37,50	1.01	4 (10%)	40,42,55	1.10	2 (5%)
45	3PE	j	101	-	39,39,50	0.97	4 (10%)	42,44,55	1.13	2 (4%)
50	FES	G	803	7	0,4,4	-	-	-	-	-
47	PLC	L	704	-	30,30,41	0.59	0	36,38,49	0.56	0
46	PC1	A	202	-	34,34,53	1.18	4 (11%)	40,42,61	1.04	2 (5%)
53	CDL	X	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
58	EHZ	U	101	20	31,36,37	1.55	5 (16%)	36,44,47	1.71	9 (25%)
59	CHD	i	201	-	32,32,32	3.27	10 (31%)	51,51,51	2.37	16 (31%)
46	PC1	H	403	-	38,38,53	1.11	4 (10%)	44,46,61	0.90	2 (4%)
49	U10	D	501	-	63,63,63	1.90	26 (41%)	78,79,79	1.61	19 (24%)
46	PC1	g	202	-	43,43,53	1.04	4 (9%)	49,51,61	1.02	2 (4%)
55	DGT	O	401	56	32,33,33	3.33	14 (43%)	48,52,52	1.95	13 (27%)
48	SF4	B	201	2	0,12,12	-	-	-	-	-
47	PLC	A	206	-	37,37,41	0.54	0	43,45,49	0.52	0
53	CDL	P	502	-	82,82,99	0.97	8 (9%)	88,94,111	1.07	4 (4%)
47	PLC	P	505	-	26,26,41	0.63	0	32,34,49	0.65	0
45	3PE	b	101	-	50,50,50	0.88	4 (8%)	53,55,55	1.15	3 (5%)
45	3PE	Y	201	-	44,44,50	0.91	4 (9%)	47,49,55	1.07	2 (4%)
45	3PE	a	101	-	35,35,50	1.02	4 (11%)	38,40,55	1.02	2 (5%)
45	3PE	N	402	-	48,48,50	0.89	4 (8%)	51,53,55	1.03	2 (3%)
46	PC1	P	503	-	45,45,53	1.03	4 (8%)	51,53,61	1.02	2 (3%)
48	SF4	F	502	6	0,12,12	-	-	-	-	-
58	EHZ	T	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.70	9 (25%)
45	3PE	Z	201	-	41,41,50	0.96	4 (9%)	44,46,55	1.09	2 (4%)
45	3PE	A	205	-	50,50,50	0.88	4 (8%)	53,55,55	1.06	2 (3%)
45	3PE	Y	208	-	50,50,50	0.88	4 (8%)	53,55,55	1.04	2 (3%)
46	PC1	d	203	-	38,38,53	1.12	4 (10%)	44,46,61	1.04	2 (4%)
45	3PE	A	201	-	46,46,50	0.91	4 (8%)	49,51,55	1.07	2 (4%)
53	CDL	i	202	-	79,79,99	0.98	8 (10%)	85,91,111	1.08	5 (5%)
47	PLC	h	201	-	31,31,41	0.57	0	37,39,49	0.54	0
50	FES	E	301	5	0,4,4	-	-	-	-	-
53	CDL	J	201	-	69,69,99	1.05	8 (11%)	75,81,111	1.15	4 (5%)
45	3PE	P	504	-	34,34,50	1.04	4 (11%)	37,39,55	1.15	2 (5%)
46	PC1	A	203	-	32,32,53	1.21	4 (12%)	38,40,61	1.07	2 (5%)
48	SF4	I	201	9	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.05	4 (5%)
45	3PE	H	402	-	40,40,50	0.97	4 (10%)	43,45,55	1.11	2 (4%)
47	PLC	d	204	-	35,35,41	0.56	0	41,43,49	0.57	0
45	3PE	Y	206	-	46,46,50	0.91	4 (8%)	49,51,55	1.07	2 (4%)
45	3PE	P	506	-	31,31,50	1.08	4 (12%)	34,36,55	1.14	2 (5%)
46	PC1	M	604	-	34,34,53	1.17	4 (11%)	40,42,61	1.06	2 (5%)
53	CDL	N	401	-	79,79,99	0.98	8 (10%)	85,91,111	1.11	4 (4%)
45	3PE	m	202	-	41,41,50	0.96	4 (9%)	44,46,55	1.13	2 (4%)
46	PC1	h	202	-	46,46,53	1.01	4 (8%)	52,54,61	1.03	2 (3%)
53	CDL	q	201	-	60,60,99	1.12	8 (13%)	66,72,111	1.12	4 (6%)
45	3PE	J	204	-	34,34,50	0.98	3 (8%)	37,39,55	1.09	1 (2%)
53	CDL	L	701	-	75,75,99	1.01	8 (10%)	81,87,111	1.11	4 (4%)
45	3PE	L	702	-	44,44,50	0.92	4 (9%)	47,49,55	1.09	2 (4%)
45	3PE	L	703	-	33,33,50	1.06	4 (12%)	36,38,55	1.12	2 (5%)
48	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	J	206	-	43,43,50	0.93	4 (9%)	46,48,55	1.09	2 (4%)
46	PC1	L	707	-	44,44,53	1.03	4 (9%)	50,52,61	1.01	2 (4%)
46	PC1	q	202	-	37,37,53	1.07	3 (8%)	43,45,61	0.96	1 (2%)
45	3PE	Y	203	-	50,50,50	0.88	4 (8%)	53,55,55	1.09	2 (3%)
46	PC1	B	203	-	47,47,53	1.01	4 (8%)	53,55,61	1.01	2 (3%)
45	3PE	q	203	-	20,20,50	1.31	4 (20%)	23,25,55	1.05	2 (8%)
51	FMN	F	501	-	33,33,33	2.78	10 (30%)	48,50,50	1.77	13 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	I	204	-	-	22/47/47/57	-
46	PC1	J	202	-	-	14/38/38/57	-
48	SF4	G	802	7	-	-	0/6/5/5
45	3PE	g	201	-	-	20/43/43/54	-
47	PLC	Y	207	-	-	12/39/39/45	-
47	PLC	B	202	-	-	16/40/40/45	-
46	PC1	I	203	-	-	15/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	H	401	-	-	27/51/51/57	-
48	SF4	I	202	9	-	-	0/6/5/5
45	3PE	M	603	-	-	19/53/53/54	-
45	3PE	Y	205	-	-	19/42/42/54	-
45	3PE	A	204	-	-	12/34/34/54	-
45	3PE	p	201	-	-	15/37/37/54	-
45	3PE	Y	202	-	-	7/26/26/54	-
45	3PE	d	202	-	-	12/52/52/54	-
47	PLC	J	205	-	-	20/41/41/45	-
60	MYR	o	201	40	-	6/12/12/13	-
45	3PE	m	201	-	-	19/44/44/54	-
45	3PE	Y	204	-	-	21/54/54/54	-
45	3PE	J	203	-	-	18/34/34/54	-
57	NDP	P	501	-	-	5/34/77/77	0/5/5/5
46	PC1	L	706	-	-	23/48/48/57	-
53	CDL	M	602	-	-	51/110/110/110	-
45	3PE	L	705	-	-	16/54/54/54	-
47	PLC	O	403	-	-	6/34/34/45	-
45	3PE	I	205	-	-	15/41/41/54	-
45	3PE	j	101	-	-	18/43/43/54	-
50	FES	G	803	7	-	-	0/1/1/1
47	PLC	L	704	-	-	14/34/34/45	-
46	PC1	A	202	-	-	14/38/38/57	-
53	CDL	X	201	-	-	46/110/110/110	-
58	EHZ	U	101	20	-	17/42/44/45	-
59	CHD	i	201	-	-	3/9/74/74	0/4/4/4
46	PC1	H	403	-	-	17/42/42/57	-
49	U10	D	501	-	-	24/63/87/87	0/1/1/1
46	PC1	g	202	-	-	22/47/47/57	-
55	DGT	O	401	56	-	8/22/34/34	0/3/3/3
48	SF4	B	201	2	-	-	0/6/5/5
47	PLC	A	206	-	-	18/41/41/45	-
53	CDL	P	502	-	-	33/93/93/110	-
47	PLC	P	505	-	-	13/29/29/45	-
45	3PE	b	101	-	-	28/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	Y	201	-	-	22/48/48/54	-
45	3PE	a	101	-	-	18/39/39/54	-
45	3PE	N	402	-	-	23/52/52/54	-
46	PC1	P	503	-	-	16/49/49/57	-
48	SF4	F	502	6	-	-	0/6/5/5
58	EHZ	T	101	20	-	12/42/44/45	-
45	3PE	Z	201	-	-	18/45/45/54	-
45	3PE	A	205	-	-	24/54/54/54	-
45	3PE	Y	208	-	-	27/54/54/54	-
46	PC1	d	203	-	-	13/42/42/57	-
45	3PE	A	201	-	-	21/50/50/54	-
53	CDL	i	202	-	-	26/90/90/110	-
47	PLC	h	201	-	-	11/34/34/45	-
50	FES	E	301	5	-	-	0/1/1/1
53	CDL	J	201	-	-	36/80/80/110	-
45	3PE	P	504	-	-	14/38/38/54	-
46	PC1	A	203	-	-	15/36/36/57	-
48	SF4	I	201	9	-	-	0/6/5/5
53	CDL	d	201	-	-	34/75/75/110	-
45	3PE	H	402	-	-	21/44/44/54	-
47	PLC	d	204	-	-	17/39/39/45	-
45	3PE	Y	206	-	-	26/50/50/54	-
45	3PE	P	506	-	-	18/35/35/54	-
46	PC1	M	604	-	-	17/38/38/57	-
53	CDL	N	401	-	-	46/90/90/110	-
45	3PE	m	202	-	-	18/45/45/54	-
46	PC1	h	202	-	-	26/50/50/57	-
53	CDL	q	201	-	-	25/71/71/110	-
45	3PE	J	204	-	-	18/37/37/54	-
53	CDL	L	701	-	-	27/86/86/110	-
45	3PE	L	702	-	-	20/48/48/54	-
45	3PE	L	703	-	-	23/37/37/54	-
48	SF4	G	801	7	-	-	0/6/5/5
45	3PE	J	206	-	-	16/47/47/54	-
46	PC1	L	707	-	-	29/48/48/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	q	202	-	-	18/40/40/57	-
45	3PE	Y	203	-	-	25/54/54/54	-
46	PC1	B	203	-	-	14/51/51/57	-
45	3PE	q	203	-	-	9/24/24/54	-
51	FMN	F	501	-	-	5/18/18/18	0/3/3/3

All (358) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	10.31	1.70	1.59
57	P	501	NDP	C2B-C1B	-9.05	1.30	1.53
59	i	201	CHD	C11-C12	9.02	1.68	1.53
55	O	401	DGT	O6-C6	8.83	1.40	1.23
57	P	501	NDP	O4B-C1B	8.56	1.61	1.42
57	P	501	NDP	O4D-C1D	8.37	1.61	1.42
57	P	501	NDP	C7N-N7N	7.68	1.55	1.33
57	P	501	NDP	C2D-C1D	-7.39	1.30	1.53
59	i	201	CHD	C16-C15	7.21	1.73	1.54
57	P	501	NDP	C6N-C5N	7.09	1.54	1.33
55	O	401	DGT	C5-N7	6.79	1.52	1.39
51	F	501	FMN	C10-N1	6.62	1.46	1.33
51	F	501	FMN	C4A-N5	6.61	1.45	1.30
57	P	501	NDP	O4D-C4D	-6.49	1.30	1.45
59	i	201	CHD	C20-C17	-6.24	1.43	1.54
57	P	501	NDP	P2B-O2B	5.71	1.69	1.59
51	F	501	FMN	C5A-N5	5.53	1.49	1.39
59	i	201	CHD	C8-C9	5.42	1.64	1.53
57	P	501	NDP	C6A-N6A	5.38	1.47	1.34
55	O	401	DGT	PB-O3A	5.28	1.65	1.59
59	i	201	CHD	O12-C12	-5.25	1.35	1.43
59	i	201	CHD	C13-C17	5.20	1.64	1.55
55	O	401	DGT	PA-O3A	5.19	1.65	1.59
57	P	501	NDP	O4B-C4B	-5.17	1.33	1.45
58	T	101	EHZ	C12-N1	5.16	1.45	1.33
55	O	401	DGT	PB-O3B	5.15	1.65	1.59
51	F	501	FMN	C2-N1	5.07	1.48	1.36
58	U	101	EHZ	C12-N1	5.05	1.45	1.33
51	F	501	FMN	C9A-N10	5.04	1.49	1.41
58	T	101	EHZ	C15-N2	4.91	1.45	1.33
58	U	101	EHZ	C15-N2	4.91	1.45	1.33
57	P	501	NDP	PN-O3	4.82	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	O	401	DGT	C2-N2	4.81	1.45	1.34
55	O	401	DGT	C2-N1	4.80	1.49	1.37
57	P	501	NDP	C2N-C3N	4.68	1.48	1.35
59	i	201	CHD	C6-C5	4.66	1.61	1.53
51	F	501	FMN	C2-N3	4.57	1.49	1.39
55	O	401	DGT	C2-N3	4.38	1.43	1.33
55	O	401	DGT	C8-N9	-4.24	1.28	1.37
59	i	201	CHD	C15-C14	4.23	1.63	1.54
57	P	501	NDP	C5A-C4A	-4.17	1.31	1.39
57	P	501	NDP	O7N-C7N	-4.13	1.14	1.24
57	P	501	NDP	C8A-N9A	-3.91	1.30	1.37
55	O	401	DGT	C4-N9	-3.89	1.28	1.38
51	F	501	FMN	C10-N10	3.81	1.45	1.37
51	F	501	FMN	C4-N3	3.80	1.46	1.38
57	P	501	NDP	O2D-C2D	3.69	1.52	1.43
59	i	201	CHD	C6-C7	3.57	1.59	1.52
57	P	501	NDP	C4N-C3N	3.38	1.56	1.50
49	D	501	U10	C4-C5	-3.27	1.39	1.48
49	D	501	U10	C3-C2	-3.04	1.40	1.48
49	D	501	U10	C51-C49	3.03	1.57	1.51
49	D	501	U10	C31-C29	3.02	1.57	1.51
49	D	501	U10	C20-C19	3.00	1.58	1.50
51	F	501	FMN	O2-C2	-2.87	1.18	1.24
53	i	202	CDL	OA6-CA4	-2.85	1.39	1.46
49	D	501	U10	C30-C29	2.82	1.57	1.50
57	P	501	NDP	C4N-C5N	2.79	1.56	1.49
49	D	501	U10	C35-C34	2.78	1.57	1.50
46	P	503	PC1	O21-C2	-2.76	1.40	1.46
53	P	502	CDL	OA6-CA4	-2.74	1.40	1.46
53	M	602	CDL	OB6-CB4	-2.74	1.40	1.46
53	q	201	CDL	OA6-CA4	-2.74	1.40	1.46
53	P	502	CDL	OB6-CB4	-2.73	1.40	1.46
46	g	202	PC1	O21-C2	-2.73	1.40	1.46
46	A	202	PC1	O21-C2	-2.72	1.40	1.46
53	q	201	CDL	OB6-CB4	-2.72	1.40	1.46
45	Y	202	3PE	O21-C2	-2.72	1.40	1.46
53	X	201	CDL	OB6-CB4	-2.72	1.40	1.46
53	L	701	CDL	OA6-CA4	-2.71	1.40	1.46
45	Y	203	3PE	O21-C2	-2.71	1.40	1.46
46	I	204	PC1	O21-C2	-2.70	1.40	1.46
53	L	701	CDL	OB6-CB4	-2.70	1.40	1.46
45	J	206	3PE	O21-C2	-2.69	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	201	3PE	O21-C2	-2.69	1.40	1.46
45	P	504	3PE	O21-C2	-2.68	1.40	1.46
46	M	604	PC1	O21-C2	-2.68	1.40	1.46
51	F	501	FMN	O4-C4	-2.68	1.18	1.23
45	J	204	3PE	O21-C2	-2.67	1.40	1.46
45	Y	205	3PE	O21-C2	-2.67	1.40	1.46
57	P	501	NDP	C5A-N7A	-2.67	1.34	1.39
45	L	703	3PE	O21-C2	-2.67	1.40	1.46
53	M	602	CDL	OA6-CA4	-2.66	1.40	1.46
53	J	201	CDL	OB6-CB4	-2.66	1.40	1.46
45	Z	201	3PE	O21-C2	-2.66	1.40	1.46
46	B	203	PC1	O21-C2	-2.66	1.40	1.46
46	L	706	PC1	O21-C2	-2.66	1.40	1.46
53	N	401	CDL	OB6-CB4	-2.66	1.40	1.46
46	A	203	PC1	O21-C2	-2.65	1.40	1.46
45	M	603	3PE	O21-C2	-2.65	1.40	1.46
53	J	201	CDL	OA6-CA4	-2.65	1.40	1.46
46	J	202	PC1	O21-C2	-2.65	1.40	1.46
55	O	401	DGT	C1'-N9	-2.64	1.41	1.48
45	g	201	3PE	O21-C2	-2.64	1.40	1.46
45	m	202	3PE	O21-C2	-2.64	1.40	1.46
45	J	203	3PE	O21-C2	-2.64	1.40	1.46
46	h	202	PC1	O21-C2	-2.64	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.64	1.40	1.46
45	I	205	3PE	O21-C2	-2.63	1.40	1.46
46	I	203	PC1	O21-C2	-2.63	1.40	1.46
45	d	202	3PE	O21-C2	-2.63	1.40	1.46
46	H	401	PC1	O21-C2	-2.62	1.40	1.46
45	A	205	3PE	O21-C2	-2.62	1.40	1.46
46	L	707	PC1	O21-C2	-2.62	1.40	1.46
46	d	203	PC1	O21-C2	-2.62	1.40	1.46
45	H	402	3PE	O21-C2	-2.62	1.40	1.46
45	N	402	3PE	O21-C2	-2.62	1.40	1.46
45	A	204	3PE	O21-C2	-2.60	1.40	1.46
45	q	203	3PE	O21-C2	-2.60	1.40	1.46
45	a	101	3PE	O21-C2	-2.60	1.40	1.46
53	d	201	CDL	OB6-CB4	-2.59	1.40	1.46
45	p	201	3PE	O21-C2	-2.59	1.40	1.46
45	m	201	3PE	O21-C2	-2.58	1.40	1.46
53	i	202	CDL	OB6-CB4	-2.57	1.40	1.46
49	D	501	U10	C41-C39	2.57	1.56	1.51
45	Y	206	3PE	O21-C2	-2.57	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	D	501	U10	C6-C1	2.56	1.39	1.35
53	M	602	CDL	OA8-CA7	2.55	1.40	1.33
57	P	501	NDP	C6N-N1N	2.55	1.43	1.37
49	D	501	U10	C15-C14	2.55	1.56	1.50
46	J	202	PC1	O31-C31	2.54	1.40	1.33
49	D	501	U10	C16-C14	2.53	1.56	1.51
45	P	506	3PE	O21-C2	-2.53	1.40	1.46
46	H	403	PC1	O21-C2	-2.53	1.40	1.46
53	L	701	CDL	OB8-CB7	2.52	1.40	1.33
45	Y	204	3PE	O21-C2	-2.51	1.40	1.46
53	J	201	CDL	OB8-CB7	2.50	1.40	1.33
45	Y	208	3PE	O21-C2	-2.50	1.40	1.46
59	i	201	CHD	C13-C12	-2.50	1.50	1.54
45	L	705	3PE	O21-C2	-2.50	1.40	1.46
53	X	201	CDL	OA6-CA4	-2.49	1.40	1.46
46	q	202	PC1	O21-C2	-2.49	1.40	1.46
53	q	201	CDL	OB8-CB7	2.48	1.40	1.33
46	L	706	PC1	O31-C31	2.47	1.40	1.33
53	X	201	CDL	OA8-CA7	2.47	1.40	1.33
53	N	401	CDL	OA8-CA7	2.45	1.40	1.33
49	D	501	U10	C7-C8	2.44	1.54	1.50
46	I	203	PC1	O31-C31	2.44	1.40	1.33
53	d	201	CDL	OB8-CB7	2.44	1.40	1.33
45	L	702	3PE	O31-C31	2.44	1.40	1.33
46	B	203	PC1	O31-C31	2.43	1.40	1.33
46	A	203	PC1	O31-C31	2.43	1.40	1.33
46	h	202	PC1	O31-C31	2.43	1.40	1.33
53	i	202	CDL	OB8-CB7	2.42	1.40	1.33
46	H	403	PC1	O31-C31	2.42	1.40	1.33
53	N	401	CDL	OA6-CA4	-2.41	1.40	1.46
53	J	201	CDL	OA8-CA7	2.41	1.40	1.33
49	D	501	U10	C40-C39	2.41	1.56	1.50
45	j	101	3PE	O31-C31	2.41	1.40	1.33
49	D	501	U10	C1M-C1	2.40	1.55	1.50
53	i	202	CDL	OA8-CA7	2.40	1.40	1.33
53	M	602	CDL	OB8-CB7	2.40	1.40	1.33
46	M	604	PC1	O31-C31	2.40	1.40	1.33
45	L	703	3PE	O31-C31	2.39	1.40	1.33
45	Z	201	3PE	O31-C31	2.39	1.40	1.33
45	q	203	3PE	O31-C31	2.39	1.40	1.33
45	m	201	3PE	O31-C31	2.39	1.40	1.33
45	L	702	3PE	O21-C2	-2.39	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	T	101	EHZ	O4-C15	-2.39	1.18	1.23
58	U	101	EHZ	O4-C15	-2.39	1.18	1.23
45	Y	201	3PE	O21-C2	-2.39	1.41	1.46
46	P	503	PC1	O31-C31	2.39	1.40	1.33
45	Y	205	3PE	O31-C31	2.39	1.40	1.33
49	D	501	U10	C50-C49	2.39	1.56	1.50
46	d	203	PC1	O31-C31	2.39	1.40	1.33
45	M	603	3PE	O31-C31	2.38	1.40	1.33
45	A	201	3PE	O31-C31	2.38	1.40	1.33
46	g	202	PC1	O31-C31	2.38	1.40	1.33
53	P	502	CDL	OB8-CB7	2.38	1.40	1.33
53	N	401	CDL	OB8-CB7	2.38	1.40	1.33
45	Y	208	3PE	O31-C31	2.38	1.40	1.33
58	T	101	EHZ	C9-S1	2.37	1.81	1.76
45	N	402	3PE	O31-C31	2.37	1.40	1.33
45	H	402	3PE	O31-C31	2.37	1.40	1.33
46	I	204	PC1	O31-C31	2.37	1.40	1.33
46	H	401	PC1	O31-C31	2.37	1.40	1.33
45	b	101	3PE	O31-C31	2.36	1.40	1.33
58	U	101	EHZ	O3-C12	-2.36	1.18	1.23
45	J	203	3PE	O31-C31	2.36	1.40	1.33
45	Y	201	3PE	O31-C31	2.36	1.40	1.33
57	P	501	NDP	O3B-C3B	-2.36	1.37	1.43
49	D	501	U10	C46-C44	2.36	1.56	1.51
53	L	701	CDL	OA8-CA7	2.36	1.40	1.33
45	b	101	3PE	O21-C2	-2.36	1.41	1.46
45	I	205	3PE	O31-C31	2.36	1.40	1.33
45	A	204	3PE	O31-C31	2.35	1.40	1.33
46	A	202	PC1	O31-C31	2.35	1.40	1.33
45	P	506	3PE	O31-C31	2.35	1.40	1.33
45	Y	204	3PE	O31-C31	2.35	1.40	1.33
45	Y	203	3PE	O31-C31	2.35	1.40	1.33
57	P	501	NDP	O3D-C3D	-2.35	1.37	1.43
45	j	101	3PE	O21-C2	-2.35	1.41	1.46
45	b	101	3PE	O21-C21	2.35	1.40	1.34
45	Y	206	3PE	O31-C31	2.34	1.40	1.33
45	d	202	3PE	O31-C31	2.34	1.40	1.33
53	P	502	CDL	OA8-CA7	2.34	1.40	1.33
57	P	501	NDP	P2B-O1X	2.34	1.57	1.50
53	d	201	CDL	OA8-CA7	2.34	1.40	1.33
45	P	504	3PE	O31-C31	2.34	1.40	1.33
58	U	101	EHZ	C9-S1	2.34	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	q	201	CDL	OA8-CA7	2.33	1.40	1.33
45	J	206	3PE	O31-C31	2.32	1.40	1.33
45	Y	202	3PE	O31-C31	2.32	1.40	1.33
53	X	201	CDL	OB8-CB6	-2.32	1.40	1.45
45	m	202	3PE	O31-C31	2.31	1.40	1.33
45	A	205	3PE	O31-C3	-2.31	1.40	1.45
49	D	501	U10	C36-C34	2.31	1.56	1.51
45	a	101	3PE	O31-C31	2.31	1.40	1.33
58	T	101	EHZ	O3-C12	-2.31	1.18	1.23
57	P	501	NDP	PA-O5B	2.30	1.68	1.59
53	P	502	CDL	OB8-CB6	-2.30	1.40	1.45
57	P	501	NDP	C7N-C3N	2.30	1.53	1.48
45	L	705	3PE	O31-C31	2.30	1.40	1.33
53	d	201	CDL	OA8-CA6	-2.30	1.40	1.45
53	X	201	CDL	OB8-CB7	2.29	1.40	1.33
45	A	205	3PE	O31-C31	2.29	1.40	1.33
45	g	201	3PE	O31-C31	2.29	1.40	1.33
53	q	201	CDL	OA8-CA6	-2.28	1.40	1.45
46	H	403	PC1	O21-C21	2.28	1.40	1.34
46	L	707	PC1	O31-C31	2.28	1.40	1.33
45	m	202	3PE	O31-C3	-2.27	1.40	1.45
55	O	401	DGT	PG-O1G	-2.26	1.46	1.54
45	g	201	3PE	O31-C3	-2.26	1.40	1.45
45	a	101	3PE	O31-C3	-2.26	1.40	1.45
45	Y	203	3PE	O31-C3	-2.26	1.40	1.45
53	d	201	CDL	OB6-CB5	2.26	1.40	1.34
46	L	707	PC1	O31-C3	-2.26	1.40	1.45
55	O	401	DGT	PG-O2G	-2.25	1.46	1.54
45	J	206	3PE	O31-C3	-2.25	1.40	1.45
46	L	707	PC1	O21-C21	2.25	1.40	1.34
45	Y	204	3PE	O21-C21	2.24	1.40	1.34
45	H	402	3PE	O31-C3	-2.23	1.40	1.45
45	M	603	3PE	O31-C3	-2.23	1.40	1.45
45	L	702	3PE	O21-C21	2.22	1.40	1.34
46	I	203	PC1	O21-C21	2.22	1.40	1.34
53	P	502	CDL	OA8-CA6	-2.22	1.40	1.45
45	Y	202	3PE	O31-C3	-2.22	1.40	1.45
46	B	203	PC1	O21-C21	2.22	1.40	1.34
45	p	201	3PE	O31-C3	-2.21	1.40	1.45
53	i	202	CDL	OA8-CA6	-2.21	1.40	1.45
53	i	202	CDL	OB6-CB5	2.21	1.40	1.34
45	Y	204	3PE	O31-C3	-2.21	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	401	PC1	O31-C3	-2.21	1.40	1.45
45	Y	208	3PE	O31-C3	-2.21	1.40	1.45
46	g	202	PC1	O31-C3	-2.21	1.40	1.45
45	Y	208	3PE	O21-C21	2.21	1.40	1.34
53	X	201	CDL	OA6-CA5	2.21	1.40	1.34
45	d	202	3PE	O31-C3	-2.21	1.40	1.45
53	d	201	CDL	OA6-CA5	2.20	1.40	1.34
46	H	401	PC1	O21-C21	2.20	1.40	1.34
55	O	401	DGT	C4-N3	2.20	1.39	1.34
45	P	504	3PE	O31-C3	-2.20	1.40	1.45
46	q	202	PC1	O31-C3	-2.20	1.40	1.45
45	A	204	3PE	O31-C3	-2.20	1.40	1.45
46	d	203	PC1	O21-C21	2.20	1.40	1.34
49	D	501	U10	C26-C24	2.20	1.55	1.51
53	M	602	CDL	OA6-CA5	2.19	1.40	1.34
49	D	501	U10	C1-C2	-2.19	1.39	1.47
53	N	401	CDL	OB6-CB5	2.19	1.40	1.34
45	P	506	3PE	O31-C3	-2.19	1.40	1.45
45	L	705	3PE	O21-C21	2.18	1.40	1.34
45	Y	206	3PE	O21-C21	2.18	1.40	1.34
46	I	204	PC1	O31-C3	-2.18	1.40	1.45
53	M	602	CDL	OB8-CB6	-2.18	1.40	1.45
53	N	401	CDL	OB8-CB6	-2.18	1.40	1.45
45	j	101	3PE	O31-C3	-2.18	1.40	1.45
45	L	705	3PE	O31-C3	-2.18	1.40	1.45
46	A	202	PC1	O31-C3	-2.18	1.40	1.45
45	L	703	3PE	O31-C3	-2.18	1.40	1.45
45	A	201	3PE	O31-C3	-2.17	1.40	1.45
45	Y	205	3PE	O31-C3	-2.17	1.40	1.45
45	Y	206	3PE	O31-C3	-2.17	1.40	1.45
45	A	205	3PE	O21-C21	2.17	1.40	1.34
45	a	101	3PE	O21-C21	2.17	1.40	1.34
45	J	204	3PE	O31-C3	-2.17	1.40	1.45
45	Z	201	3PE	O31-C3	-2.17	1.40	1.45
46	J	202	PC1	O21-C21	2.17	1.40	1.34
45	m	201	3PE	O31-C3	-2.17	1.40	1.45
45	b	101	3PE	O31-C3	-2.17	1.40	1.45
53	N	401	CDL	OA6-CA5	2.16	1.40	1.34
53	L	701	CDL	OB6-CB5	2.16	1.40	1.34
45	p	201	3PE	O21-C21	2.16	1.40	1.34
46	L	706	PC1	O21-C21	2.16	1.40	1.34
46	h	202	PC1	O31-C3	-2.16	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	P	506	3PE	O21-C21	2.16	1.40	1.34
53	J	201	CDL	OA8-CA6	-2.16	1.40	1.45
46	H	403	PC1	O31-C3	-2.16	1.40	1.45
45	m	202	3PE	O21-C21	2.16	1.40	1.34
46	P	503	PC1	O31-C3	-2.16	1.40	1.45
53	d	201	CDL	OB8-CB6	-2.16	1.40	1.45
45	g	201	3PE	O21-C21	2.15	1.40	1.34
45	j	101	3PE	O21-C21	2.15	1.40	1.34
45	J	203	3PE	O31-C3	-2.15	1.40	1.45
46	d	203	PC1	O31-C3	-2.15	1.40	1.45
49	D	501	U10	O4-C4	2.15	1.42	1.36
46	A	203	PC1	O31-C3	-2.15	1.40	1.45
46	A	203	PC1	O21-C21	2.15	1.40	1.34
45	q	203	3PE	O31-C3	-2.15	1.40	1.45
49	D	501	U10	C25-C24	2.15	1.56	1.50
45	A	204	3PE	O21-C21	2.15	1.40	1.34
45	I	205	3PE	O21-C21	2.15	1.40	1.34
45	m	201	3PE	O21-C21	2.15	1.40	1.34
45	I	205	3PE	O31-C3	-2.15	1.40	1.45
46	M	604	PC1	O31-C3	-2.14	1.40	1.45
57	P	501	NDP	C5B-C4B	2.14	1.58	1.51
45	N	402	3PE	O31-C3	-2.14	1.40	1.45
45	L	702	3PE	O31-C3	-2.14	1.40	1.45
46	q	202	PC1	O21-C21	2.14	1.40	1.34
45	J	204	3PE	O21-C21	2.14	1.40	1.34
45	N	402	3PE	O21-C21	2.14	1.40	1.34
46	h	202	PC1	O21-C21	2.14	1.40	1.34
53	q	201	CDL	OB6-CB5	2.14	1.40	1.34
53	J	201	CDL	OB6-CB5	2.13	1.40	1.34
46	I	203	PC1	O31-C3	-2.13	1.40	1.45
53	N	401	CDL	OA8-CA6	-2.13	1.40	1.45
53	q	201	CDL	OA6-CA5	2.13	1.40	1.34
49	D	501	U10	O3-C3	2.13	1.41	1.36
45	J	203	3PE	O21-C21	2.13	1.40	1.34
53	P	502	CDL	OB6-CB5	2.12	1.40	1.34
46	A	202	PC1	O21-C21	2.12	1.40	1.34
45	q	203	3PE	O21-C21	2.12	1.40	1.34
45	Y	202	3PE	O21-C21	2.12	1.40	1.34
53	L	701	CDL	OA8-CA6	-2.12	1.40	1.45
46	g	202	PC1	O21-C21	2.12	1.40	1.34
53	i	202	CDL	OB8-CB6	-2.12	1.40	1.45
46	I	204	PC1	O21-C21	2.11	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	d	202	3PE	O21-C21	2.11	1.40	1.34
45	Y	201	3PE	O21-C21	2.11	1.40	1.34
45	J	206	3PE	O21-C21	2.11	1.40	1.34
45	M	603	3PE	O21-C21	2.11	1.40	1.34
53	J	201	CDL	OA6-CA5	2.11	1.40	1.34
45	Y	201	3PE	O31-C3	-2.11	1.40	1.45
45	L	703	3PE	O21-C21	2.11	1.40	1.34
45	P	504	3PE	O21-C21	2.11	1.40	1.34
49	D	501	U10	C6-C5	-2.10	1.40	1.46
45	A	201	3PE	O21-C21	2.10	1.40	1.34
49	D	501	U10	C10-C9	2.10	1.55	1.50
45	Z	201	3PE	O21-C21	2.10	1.40	1.34
53	q	201	CDL	OB8-CB6	-2.10	1.40	1.45
46	L	706	PC1	O31-C3	-2.09	1.40	1.45
45	H	402	3PE	O21-C21	2.09	1.40	1.34
53	L	701	CDL	OA6-CA5	2.09	1.40	1.34
46	M	604	PC1	O21-C21	2.09	1.40	1.34
53	J	201	CDL	OB8-CB6	-2.09	1.40	1.45
53	M	602	CDL	OA8-CA6	-2.08	1.40	1.45
53	P	502	CDL	OA6-CA5	2.08	1.40	1.34
53	M	602	CDL	OB6-CB5	2.08	1.40	1.34
53	X	201	CDL	OB6-CB5	2.08	1.40	1.34
53	L	701	CDL	OB8-CB6	-2.07	1.40	1.45
46	P	503	PC1	O21-C21	2.06	1.40	1.34
45	Y	203	3PE	O21-C21	2.05	1.40	1.34
49	D	501	U10	C11-C9	2.05	1.55	1.51
45	Y	205	3PE	O21-C21	2.05	1.40	1.34
49	D	501	U10	C7-C6	2.04	1.55	1.51
53	i	202	CDL	OA6-CA5	2.04	1.40	1.34
46	J	202	PC1	O31-C3	-2.02	1.40	1.45
53	X	201	CDL	OA8-CA6	-2.01	1.40	1.45
46	B	203	PC1	O31-C3	-2.00	1.40	1.45

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	C8-N9-C4	7.44	119.97	106.03
59	i	201	CHD	C13-C17-C20	-7.43	110.48	119.48
58	T	101	EHZ	C8-C9-S1	5.97	121.09	113.56
57	P	501	NDP	N6A-C6A-N1A	-5.52	106.08	118.38
57	P	501	NDP	C4A-N9A-C1B	-5.52	113.72	126.63
57	P	501	NDP	N3A-C2A-N1A	-5.51	120.24	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	i	201	CHD	C17-C13-C14	5.50	105.63	100.11
59	i	201	CHD	C14-C13-C12	5.43	112.38	107.42
58	U	101	EHZ	C8-C9-S1	5.34	120.30	113.56
45	b	101	3PE	O21-C21-C22	5.09	122.49	111.48
57	P	501	NDP	C1B-N9A-C8A	4.98	138.16	127.09
59	i	201	CHD	C17-C13-C12	4.98	122.15	117.67
57	P	501	NDP	C5A-C4A-N3A	-4.94	119.91	126.72
51	F	501	FMN	C7M-C7-C6	4.78	127.99	119.57
51	F	501	FMN	C9-C8-C7	4.61	126.46	119.69
46	H	401	PC1	O21-C21-C22	4.35	120.88	111.48
53	M	602	CDL	OA6-CA5-C11	4.31	120.80	111.48
45	p	201	3PE	O21-C21-C22	4.24	120.64	111.48
45	L	705	3PE	O21-C21-C22	4.20	120.57	111.48
49	D	501	U10	C40-C39-C41	4.19	122.50	115.23
59	i	201	CHD	C18-C13-C12	-4.18	104.87	109.06
45	N	402	3PE	O21-C21-C22	4.18	120.51	111.48
45	Y	201	3PE	O21-C21-C22	4.16	120.48	111.48
45	L	702	3PE	O21-C21-C22	4.16	120.48	111.48
45	H	402	3PE	O21-C21-C22	4.14	120.44	111.48
45	m	202	3PE	O21-C21-C22	4.12	120.40	111.48
45	j	101	3PE	O21-C21-C22	4.12	120.39	111.48
45	g	201	3PE	O21-C21-C22	4.08	120.30	111.48
57	P	501	NDP	C5A-C6A-N6A	4.07	133.36	123.29
53	M	602	CDL	OB6-CB5-C51	4.07	120.28	111.48
53	i	202	CDL	OB6-CB5-C51	4.06	120.27	111.48
45	m	201	3PE	O21-C21-C22	4.05	120.25	111.48
45	Y	202	3PE	O21-C21-C22	4.05	120.24	111.48
53	X	201	CDL	OB6-CB5-C51	4.05	120.24	111.48
45	L	703	3PE	O21-C21-C22	4.04	120.22	111.48
53	J	201	CDL	OA6-CA5-C11	4.03	120.20	111.48
59	i	201	CHD	C18-C13-C17	-4.02	104.90	111.20
53	J	201	CDL	OB6-CB5-C51	4.01	120.15	111.48
45	Y	203	3PE	O21-C21-C22	4.01	120.15	111.48
45	A	205	3PE	O21-C21-C22	4.00	120.12	111.48
45	Y	205	3PE	O21-C21-C22	3.99	120.12	111.48
57	P	501	NDP	N9A-C8A-N7A	-3.99	108.28	113.94
46	A	203	PC1	O21-C21-C22	3.97	120.07	111.48
53	L	701	CDL	OA6-CA5-C11	3.97	120.06	111.48
46	L	706	PC1	O21-C21-C22	3.96	120.04	111.48
45	Y	206	3PE	O21-C21-C22	3.95	120.03	111.48
53	N	401	CDL	OA6-CA5-C11	3.95	120.02	111.48
45	P	504	3PE	O21-C21-C22	3.94	120.01	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	N	401	CDL	OB6-CB5-C51	3.94	120.00	111.48
45	Y	208	3PE	O21-C21-C22	3.93	119.98	111.48
45	I	205	3PE	O21-C21-C22	3.92	119.97	111.48
46	B	203	PC1	O21-C21-C22	3.92	119.95	111.48
53	P	502	CDL	OA6-CA5-C11	3.91	119.95	111.48
45	J	204	3PE	O21-C21-C22	3.91	119.93	111.48
45	Z	201	3PE	O21-C21-C22	3.90	119.91	111.48
45	J	203	3PE	O21-C21-C22	3.90	119.91	111.48
46	M	604	PC1	O21-C21-C22	3.89	119.90	111.48
45	d	202	3PE	O21-C21-C22	3.89	119.90	111.48
45	A	204	3PE	O21-C21-C22	3.89	119.89	111.48
46	d	203	PC1	O21-C21-C22	3.89	119.89	111.48
53	q	201	CDL	OA6-CA5-C11	3.88	119.89	111.48
53	L	701	CDL	OB6-CB5-C51	3.88	119.88	111.48
45	P	506	3PE	O21-C21-C22	3.88	119.88	111.48
53	X	201	CDL	OA6-CA5-C11	3.87	119.86	111.48
46	h	202	PC1	O21-C21-C22	3.86	119.83	111.48
46	L	707	PC1	O21-C21-C22	3.85	119.80	111.48
46	J	202	PC1	O21-C21-C22	3.84	119.78	111.48
53	i	202	CDL	OA6-CA5-C11	3.83	119.77	111.48
46	I	203	PC1	O21-C21-C22	3.79	119.68	111.48
53	d	201	CDL	OA6-CA5-C11	3.77	119.64	111.48
45	Y	204	3PE	O21-C21-C22	3.75	119.58	111.48
46	g	202	PC1	O21-C21-C22	3.75	119.58	111.48
46	A	202	PC1	O21-C21-C22	3.74	119.57	111.48
45	A	201	3PE	O21-C21-C22	3.73	119.56	111.48
53	P	502	CDL	OB6-CB5-C51	3.70	119.49	111.48
46	q	202	PC1	O21-C21-C22	3.69	119.47	111.48
53	q	201	CDL	OB6-CB5-C51	3.69	119.46	111.48
46	I	204	PC1	O21-C21-C22	3.67	119.43	111.48
46	P	503	PC1	O21-C21-C22	3.66	119.40	111.48
45	M	603	3PE	O21-C21-C22	3.65	119.37	111.48
45	J	206	3PE	O21-C21-C22	3.64	119.36	111.48
59	i	201	CHD	C18-C13-C14	-3.60	105.56	111.20
55	O	401	DGT	C1'-N9-C8	-3.59	119.87	127.91
59	i	201	CHD	C1-C10-C5	3.52	112.80	107.75
49	D	501	U10	C7-C8-C9	3.48	132.83	126.83
51	F	501	FMN	C4-N3-C2	-3.44	119.53	125.64
57	P	501	NDP	C2A-N3A-C4A	3.42	120.19	111.83
53	M	602	CDL	OA8-CA7-C31	3.41	122.22	111.83
51	F	501	FMN	C8M-C8-C7	-3.23	114.17	120.76
49	D	501	U10	C17-C18-C19	3.22	135.00	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	D	501	U10	C45-C44-C46	3.18	120.75	115.23
55	O	401	DGT	C2-N1-C6	-3.18	119.35	125.11
49	D	501	U10	C10-C9-C11	3.17	120.73	115.23
49	D	501	U10	C15-C14-C16	3.10	120.61	115.23
55	O	401	DGT	C2'-C3'-C4'	3.07	109.03	102.80
49	D	501	U10	C22-C23-C24	-3.06	120.63	127.62
57	P	501	NDP	N3A-C4A-N9A	3.04	132.34	127.17
59	i	201	CHD	C6-C5-C4	-3.00	107.80	111.23
53	L	701	CDL	OA8-CA7-C31	2.98	120.93	111.83
53	X	201	CDL	OA8-CA7-C31	2.97	120.90	111.83
49	D	501	U10	C20-C19-C18	-2.94	116.07	123.63
49	D	501	U10	C30-C29-C31	2.94	120.33	115.23
53	J	201	CDL	OB8-CB7-C71	2.93	120.77	111.83
49	D	501	U10	C32-C33-C34	2.91	134.29	127.62
45	Y	203	3PE	O31-C31-C32	2.87	120.57	111.83
45	Y	206	3PE	O31-C31-C32	2.85	120.54	111.83
45	Y	204	3PE	O31-C31-C32	2.85	120.53	111.83
55	O	401	DGT	O2G-PG-O3B	2.84	114.17	104.64
46	h	202	PC1	O31-C31-C32	2.84	120.51	111.83
45	J	206	3PE	O31-C31-C32	2.84	120.48	111.83
45	P	506	3PE	O31-C31-C32	2.81	120.40	111.83
46	A	202	PC1	O31-C31-C32	2.80	120.37	111.83
53	N	401	CDL	OA8-CA7-C31	2.79	120.35	111.83
45	Y	208	3PE	O31-C31-C32	2.79	120.34	111.83
46	d	203	PC1	O31-C31-C32	2.79	120.34	111.83
59	i	201	CHD	C15-C14-C8	2.79	122.18	118.36
45	Y	205	3PE	O31-C31-C32	2.79	120.33	111.83
46	L	706	PC1	O31-C31-C32	2.78	120.32	111.83
53	P	502	CDL	OA8-CA7-C31	2.78	120.31	111.83
53	d	201	CDL	OB8-CB7-C71	2.78	120.30	111.83
49	D	501	U10	C25-C24-C26	2.77	120.03	115.23
46	H	403	PC1	O31-C31-C32	2.75	120.23	111.83
45	A	201	3PE	O31-C31-C32	2.75	120.23	111.83
53	M	602	CDL	OB8-CB7-C71	2.75	120.21	111.83
55	O	401	DGT	O1G-PG-O3B	2.74	113.84	104.64
46	P	503	PC1	O31-C31-C32	2.74	120.20	111.83
46	A	203	PC1	O31-C31-C32	2.74	120.18	111.83
46	L	707	PC1	O31-C31-C32	2.73	120.16	111.83
53	d	201	CDL	OA8-CA7-C31	2.73	120.14	111.83
45	a	101	3PE	O31-C31-C32	2.72	120.14	111.83
45	L	705	3PE	O31-C31-C32	2.72	120.14	111.83
51	F	501	FMN	C4A-C10-N10	2.72	120.37	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	F	501	FMN	C6-C7-C8	-2.71	115.71	119.69
45	q	203	3PE	O31-C31-C32	2.70	119.36	111.15
45	P	504	3PE	O31-C31-C32	2.70	120.07	111.83
45	L	702	3PE	O31-C31-C32	2.69	120.05	111.83
46	g	202	PC1	O31-C31-C32	2.69	120.04	111.83
45	Z	201	3PE	O31-C31-C32	2.69	120.03	111.83
57	P	501	NDP	C5A-N7A-C8A	2.69	107.67	103.45
53	q	201	CDL	OB8-CB7-C71	2.69	120.03	111.83
45	J	203	3PE	O31-C31-C32	2.68	120.01	111.83
46	I	204	PC1	O31-C31-C32	2.68	120.00	111.83
45	m	202	3PE	O31-C31-C32	2.67	119.99	111.83
45	j	101	3PE	O31-C31-C32	2.67	119.98	111.83
45	I	205	3PE	O31-C31-C32	2.67	119.97	111.83
46	M	604	PC1	O31-C31-C32	2.67	119.97	111.83
53	X	201	CDL	OB8-CB7-C71	2.67	119.97	111.83
58	T	101	EHZ	O2-C9-C8	-2.66	119.55	123.74
45	M	603	3PE	O31-C31-C32	2.66	119.94	111.83
45	A	204	3PE	O31-C31-C32	2.66	119.93	111.83
53	L	701	CDL	OB8-CB7-C71	2.65	119.93	111.83
53	i	202	CDL	OB8-CB7-C71	2.65	119.90	111.83
46	H	401	PC1	O31-C31-C32	2.64	119.90	111.83
58	U	101	EHZ	C13-C12-N1	2.64	121.15	116.34
45	Y	201	3PE	O31-C31-C32	2.63	119.87	111.83
53	J	201	CDL	OA8-CA7-C31	2.63	119.86	111.83
58	T	101	EHZ	C14-C13-C12	-2.63	108.01	112.39
45	g	201	3PE	O31-C31-C32	2.63	119.86	111.83
58	U	101	EHZ	C19-C17-C16	2.62	113.24	108.77
58	T	101	EHZ	O2-C9-S1	-2.62	119.35	122.68
45	m	201	3PE	O31-C31-C32	2.62	119.81	111.83
45	A	205	3PE	O31-C31-C32	2.61	119.80	111.83
49	D	501	U10	C35-C34-C33	-2.61	116.92	123.63
51	F	501	FMN	C5A-C9A-N10	2.61	120.32	117.97
45	L	703	3PE	O31-C31-C32	2.60	119.78	111.83
49	D	501	U10	C50-C49-C51	2.60	119.74	115.23
45	Y	202	3PE	O31-C31-C32	2.60	119.76	111.83
45	H	402	3PE	O31-C31-C32	2.60	119.75	111.83
45	a	101	3PE	O21-C21-C22	2.58	120.42	110.93
59	i	201	CHD	C23-C22-C20	-2.57	109.66	114.46
45	d	202	3PE	O31-C31-C32	2.55	119.60	111.83
53	N	401	CDL	OB8-CB7-C71	2.54	119.59	111.83
51	F	501	FMN	C4A-C4-N3	2.54	119.71	113.25
45	q	203	3PE	O21-C21-C22	2.53	120.22	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	P	502	CDL	OB8-CB7-C71	2.52	119.53	111.83
46	B	203	PC1	O31-C31-C32	2.51	119.50	111.83
53	i	202	CDL	OA8-CA7-C31	2.51	119.48	111.83
51	F	501	FMN	O4-C4-C4A	-2.50	119.92	126.53
53	q	201	CDL	OA8-CA7-C31	2.50	119.45	111.83
45	b	101	3PE	O31-C31-C32	2.49	119.42	111.83
51	F	501	FMN	C9A-C5A-N5	-2.47	119.83	122.45
57	P	501	NDP	C2B-C1B-N9A	-2.47	109.69	113.75
58	U	101	EHZ	O2-C9-C8	-2.47	119.86	123.74
46	I	203	PC1	O31-C31-C32	2.46	119.34	111.83
55	O	401	DGT	C5-C6-N1	2.46	119.51	113.25
55	O	401	DGT	O1A-PA-O2A	-2.45	101.06	112.44
55	O	401	DGT	O1B-PB-O2B	-2.45	101.06	112.44
58	T	101	EHZ	C7-C8-C9	-2.44	108.41	113.86
45	N	402	3PE	O31-C31-C32	2.43	119.25	111.83
58	T	101	EHZ	C13-C14-N2	-2.43	106.83	112.00
59	i	201	CHD	C19-C10-C9	-2.42	107.92	111.18
58	U	101	EHZ	C14-C13-C12	-2.41	108.38	112.39
46	J	202	PC1	O31-C31-C32	2.38	119.09	111.83
49	D	501	U10	C15-C14-C13	-2.35	117.59	123.63
55	O	401	DGT	O6-C6-C5	-2.34	120.35	126.53
53	d	201	CDL	OB6-CB5-C51	2.32	119.46	110.93
59	i	201	CHD	C21-C20-C17	-2.28	109.45	112.88
49	D	501	U10	C7-C6-C1	-2.28	120.97	124.89
46	H	403	PC1	O21-C21-C22	2.28	119.30	110.93
57	P	501	NDP	C4A-N9A-C8A	2.27	108.12	105.74
49	D	501	U10	C56-C54-C55	2.27	119.81	114.59
51	F	501	FMN	C10-C4A-N5	-2.25	120.21	124.81
49	D	501	U10	C40-C39-C38	-2.25	117.84	123.63
58	U	101	EHZ	C7-C8-C9	-2.25	108.84	113.86
58	U	101	EHZ	O2-C9-S1	-2.24	119.83	122.68
58	U	101	EHZ	C11-N1-C12	-2.22	118.69	122.82
51	F	501	FMN	C6-C5A-C9A	2.19	122.06	119.05
51	F	501	FMN	C7M-C7-C8	-2.19	116.29	120.76
55	O	401	DGT	C5-C4-N9	-2.18	101.75	105.66
59	i	201	CHD	C9-C11-C12	-2.17	111.46	114.29
58	T	101	EHZ	C13-C12-N1	2.16	120.28	116.34
55	O	401	DGT	N9-C4-N3	2.16	130.28	125.95
59	i	201	CHD	C4-C3-C2	2.16	113.25	110.62
58	U	101	EHZ	C10-S1-C9	2.14	108.16	101.84
59	i	201	CHD	C1-C2-C3	2.13	113.30	110.48
45	b	101	3PE	O21-C21-O22	-2.12	118.76	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	P	501	NDP	C4A-C5A-N7A	-2.11	108.17	110.58
49	D	501	U10	C52-C53-C54	-2.07	120.73	127.64
49	D	501	U10	C21-C19-C18	2.07	125.82	121.17
58	T	101	EHZ	C19-C17-C16	2.05	112.26	108.77
55	O	401	DGT	N9-C8-N7	-2.04	109.62	113.40
58	T	101	EHZ	C10-S1-C9	2.03	107.85	101.84
57	P	501	NDP	P2B-O2B-C2B	-2.02	118.03	123.43
53	i	202	CDL	CA4-OA6-CA5	-2.02	112.97	117.80
57	P	501	NDP	C3N-C2N-N1N	-2.01	120.25	123.20

There are no chirality outliers.

All (1433) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	O13-C11-C12-N
45	A	204	3PE	C11-O13-P-O11
45	A	204	3PE	C11-O13-P-O12
45	A	204	3PE	O21-C2-C3-O31
45	A	205	3PE	O22-C21-O21-C2
45	H	402	3PE	C11-O13-P-O11
45	H	402	3PE	C11-O13-P-O12
45	H	402	3PE	C11-O13-P-O14
45	J	203	3PE	C11-O13-P-O11
45	J	203	3PE	C11-O13-P-O12
45	J	203	3PE	C11-O13-P-O14
45	J	204	3PE	C11-O13-P-O11
45	J	204	3PE	C11-O13-P-O12
45	J	204	3PE	C11-O13-P-O14
45	J	204	3PE	O13-C11-C12-N
45	J	206	3PE	O13-C11-C12-N
45	L	702	3PE	O13-C11-C12-N
45	L	702	3PE	C22-C21-O21-C2
45	L	703	3PE	C11-O13-P-O11
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	703	3PE	O11-C1-C2-O21
45	L	703	3PE	C22-C21-O21-C2
45	L	705	3PE	O22-C21-O21-C2
45	L	705	3PE	C22-C21-O21-C2
45	M	603	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	M	603	3PE	C11-O13-P-O14
45	M	603	3PE	C12-C11-O13-P
45	M	603	3PE	O11-C1-C2-O21
45	N	402	3PE	O13-C11-C12-N
45	N	402	3PE	O11-C1-C2-O21
45	P	506	3PE	C12-C11-O13-P
45	P	506	3PE	O13-C11-C12-N
45	P	506	3PE	C22-C21-O21-C2
45	Y	201	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O12
45	Y	201	3PE	C11-O13-P-O14
45	Y	201	3PE	O13-C11-C12-N
45	Y	201	3PE	C22-C21-O21-C2
45	Y	202	3PE	C22-C21-O21-C2
45	Y	203	3PE	C11-O13-P-O11
45	Y	204	3PE	C1-O11-P-O13
45	Y	205	3PE	C11-O13-P-O14
45	Y	205	3PE	O11-C1-C2-O21
45	Y	205	3PE	O32-C31-O31-C3
45	Y	205	3PE	O22-C21-O21-C2
45	Y	206	3PE	C12-C11-O13-P
45	Y	208	3PE	C1-O11-P-O12
45	Y	208	3PE	C1-O11-P-O13
45	Y	208	3PE	C1-O11-P-O14
45	Y	208	3PE	C11-O13-P-O11
45	Y	208	3PE	C11-O13-P-O12
45	Y	208	3PE	C11-O13-P-O14
45	Y	208	3PE	O13-C11-C12-N
45	Y	208	3PE	C22-C21-O21-C2
45	Z	201	3PE	O13-C11-C12-N
45	a	101	3PE	O22-C21-O21-C2
45	b	101	3PE	C1-O11-P-O13
45	b	101	3PE	C11-O13-P-O11
45	b	101	3PE	C11-O13-P-O12
45	b	101	3PE	O13-C11-C12-N
45	b	101	3PE	O22-C21-O21-C2
45	b	101	3PE	C22-C21-O21-C2
45	d	202	3PE	C11-O13-P-O11
45	d	202	3PE	C11-O13-P-O14
45	g	201	3PE	O13-C11-C12-N
45	g	201	3PE	O22-C21-O21-C2
45	g	201	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	j	101	3PE	C11-O13-P-O14
45	j	101	3PE	C22-C21-O21-C2
45	m	201	3PE	O13-C11-C12-N
45	m	202	3PE	O22-C21-O21-C2
45	m	202	3PE	C22-C21-O21-C2
45	p	201	3PE	C1-O11-P-O12
45	p	201	3PE	C1-O11-P-O14
45	p	201	3PE	O22-C21-O21-C2
45	q	203	3PE	C11-O13-P-O11
45	q	203	3PE	O22-C21-O21-C2
46	A	202	PC1	C1-O11-P-O14
46	A	202	PC1	C1-O11-P-O13
46	A	203	PC1	C11-O13-P-O12
46	A	203	PC1	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O11
46	A	203	PC1	O22-C21-O21-C2
46	A	203	PC1	C22-C21-O21-C2
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C11-O13-P-O11
46	B	203	PC1	O22-C21-O21-C2
46	H	401	PC1	C11-O13-P-O12
46	H	401	PC1	C11-O13-P-O11
46	H	401	PC1	C1-O11-P-O12
46	H	401	PC1	C1-O11-P-O13
46	H	401	PC1	O13-C11-C12-N
46	I	203	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O14
46	I	204	PC1	O11-C1-C2-O21
46	J	202	PC1	C11-O13-P-O12
46	J	202	PC1	C11-O13-P-O11
46	J	202	PC1	C1-O11-P-O12
46	J	202	PC1	C1-O11-P-O14
46	J	202	PC1	C1-O11-P-O13
46	J	202	PC1	O13-C11-C12-N
46	J	202	PC1	C22-C21-O21-C2
46	L	706	PC1	C11-O13-P-O12
46	L	706	PC1	C11-O13-P-O14
46	L	706	PC1	C11-O13-P-O11
46	L	706	PC1	C1-O11-P-O12
46	L	706	PC1	C1-O11-P-O14
46	L	706	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	L	706	PC1	C22-C21-O21-C2
46	L	707	PC1	C11-O13-P-O12
46	L	707	PC1	C11-O13-P-O11
46	L	707	PC1	O13-C11-C12-N
46	M	604	PC1	C11-O13-P-O12
46	M	604	PC1	C11-O13-P-O14
46	M	604	PC1	C11-O13-P-O11
46	M	604	PC1	C1-O11-P-O12
46	M	604	PC1	C1-O11-P-O14
46	M	604	PC1	C1-O11-P-O13
46	M	604	PC1	C22-C21-O21-C2
46	d	203	PC1	C1-O11-P-O12
46	d	203	PC1	C1-O11-P-O14
46	d	203	PC1	C1-O11-P-O13
46	g	202	PC1	C1-O11-P-O12
46	g	202	PC1	C1-O11-P-O14
46	g	202	PC1	C1-O11-P-O13
46	h	202	PC1	C11-O13-P-O14
46	h	202	PC1	C11-O13-P-O11
46	h	202	PC1	C1-O11-P-O12
46	q	202	PC1	C11-O13-P-O14
46	q	202	PC1	C1-O11-P-O12
46	q	202	PC1	C1-O11-P-O13
46	q	202	PC1	C2-C1-O11-P
46	q	202	PC1	O21-C2-C3-O31
47	A	206	PLC	C1'-C'-O2-C2
47	A	206	PLC	C1-O3P-P-O1P
47	A	206	PLC	C1-O3P-P-O2P
47	A	206	PLC	C1-O3P-P-O4P
47	A	206	PLC	C4-O4P-P-O3P
47	B	202	PLC	O'-C'-O2-C2
47	B	202	PLC	C1-O3P-P-O1P
47	B	202	PLC	C1-O3P-P-O2P
47	B	202	PLC	C1-O3P-P-O4P
47	B	202	PLC	C4-O4P-P-O1P
47	B	202	PLC	C4-O4P-P-O2P
47	B	202	PLC	C4-O4P-P-O3P
47	J	205	PLC	C1'-C'-O2-C2
47	J	205	PLC	C4-O4P-P-O1P
47	J	205	PLC	C4-O4P-P-O2P
47	J	205	PLC	C4-O4P-P-O3P
47	L	704	PLC	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
47	L	704	PLC	O4P-C4-C5-N
47	L	704	PLC	C1-O3P-P-O2P
47	P	505	PLC	C1-O3P-P-O1P
47	P	505	PLC	C1-O3P-P-O4P
47	P	505	PLC	C4-O4P-P-O1P
47	P	505	PLC	C4-O4P-P-O3P
47	Y	207	PLC	O4P-C4-C5-N
47	Y	207	PLC	C5-C4-O4P-P
47	Y	207	PLC	C4-O4P-P-O1P
47	Y	207	PLC	C4-O4P-P-O3P
47	d	204	PLC	O3P-C1-C2-O2
47	d	204	PLC	O4P-C4-C5-N
47	d	204	PLC	C1'-C'-O2-C2
47	d	204	PLC	C1-O3P-P-O2P
47	d	204	PLC	C1-O3P-P-O4P
49	D	501	U10	C16-C17-C18-C19
49	D	501	U10	C31-C32-C33-C34
51	F	501	FMN	C5'-O5'-P-O1P
53	J	201	CDL	O1-C1-CA2-OA2
53	J	201	CDL	CA3-OA5-PA1-OA2
53	J	201	CDL	C11-CA5-OA6-CA4
53	J	201	CDL	C1-CB2-OB2-PB2
53	J	201	CDL	CB3-OB5-PB2-OB2
53	J	201	CDL	CB3-OB5-PB2-OB3
53	J	201	CDL	OB7-CB5-OB6-CB4
53	L	701	CDL	CA3-OA5-PA1-OA2
53	L	701	CDL	CA3-OA5-PA1-OA3
53	L	701	CDL	CB2-OB2-PB2-OB3
53	L	701	CDL	CB3-OB5-PB2-OB2
53	L	701	CDL	CB3-OB5-PB2-OB3
53	M	602	CDL	C1-CA2-OA2-PA1
53	M	602	CDL	CA2-OA2-PA1-OA4
53	M	602	CDL	CA2-OA2-PA1-OA5
53	M	602	CDL	CA3-OA5-PA1-OA2
53	M	602	CDL	CA3-OA5-PA1-OA3
53	M	602	CDL	CA3-OA5-PA1-OA4
53	M	602	CDL	C11-CA5-OA6-CA4
53	M	602	CDL	OB5-CB3-CB4-OB6
53	M	602	CDL	OB7-CB5-OB6-CB4
53	M	602	CDL	C51-CB5-OB6-CB4
53	N	401	CDL	C11-CA5-OA6-CA4
53	N	401	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
53	P	502	CDL	C11-CA5-OA6-CA4
53	P	502	CDL	CB2-OB2-PB2-OB5
53	X	201	CDL	C11-CA5-OA6-CA4
53	X	201	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	C51-CB5-OB6-CB4
53	d	201	CDL	CA3-OA5-PA1-OA2
53	d	201	CDL	CA3-OA5-PA1-OA3
53	d	201	CDL	CB2-OB2-PB2-OB3
53	d	201	CDL	CB2-OB2-PB2-OB5
53	d	201	CDL	CB3-OB5-PB2-OB2
53	d	201	CDL	CB3-OB5-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB4
53	i	202	CDL	C11-CA5-OA6-CA4
53	i	202	CDL	CB3-OB5-PB2-OB3
53	i	202	CDL	OB7-CB5-OB6-CB4
53	i	202	CDL	OB9-CB7-OB8-CB6
53	q	201	CDL	C11-CA5-OA6-CA4
53	q	201	CDL	CB3-OB5-PB2-OB2
53	q	201	CDL	CB3-OB5-PB2-OB3
53	q	201	CDL	CB3-OB5-PB2-OB4
55	O	401	DGT	PB-O3B-PG-O1G
55	O	401	DGT	C5'-O5'-PA-O3A
55	O	401	DGT	C5'-O5'-PA-O1A
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	O2-C9-S1-C10
58	T	101	EHZ	C8-C9-S1-C10
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	S1-C10-C11-N1
58	U	101	EHZ	C15-C16-C17-C18
58	U	101	EHZ	C15-C16-C17-C19
58	U	101	EHZ	C15-C16-C17-C20
58	U	101	EHZ	O5-C16-C17-C18
58	U	101	EHZ	O5-C16-C17-C19
58	U	101	EHZ	O5-C16-C17-C20
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
60	o	201	MYR	O1-C1-C2-C3
45	J	203	3PE	O32-C31-O31-C3
46	L	706	PC1	O32-C31-O31-C3
53	J	201	CDL	OB9-CB7-OB8-CB6
53	M	602	CDL	OA9-CA7-OA8-CA6
45	Y	203	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	j	101	3PE	C32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
53	J	201	CDL	C71-CB7-OB8-CB6
53	M	602	CDL	C31-CA7-OA8-CA6
53	i	202	CDL	C71-CB7-OB8-CB6
45	A	205	3PE	O32-C31-O31-C3
45	P	504	3PE	O32-C31-O31-C3
45	Y	203	3PE	O32-C31-O31-C3
45	Y	204	3PE	O32-C31-O31-C3
45	Y	206	3PE	O32-C31-O31-C3
45	j	101	3PE	O32-C31-O31-C3
45	m	201	3PE	O32-C31-O31-C3
46	H	403	PC1	O32-C31-O31-C3
46	d	203	PC1	O32-C31-O31-C3
46	g	202	PC1	O32-C31-O31-C3
46	h	202	PC1	O32-C31-O31-C3
53	M	602	CDL	OB9-CB7-OB8-CB6
53	N	401	CDL	OA9-CA7-OA8-CA6
53	d	201	CDL	OB9-CB7-OB8-CB6
45	L	703	3PE	O22-C21-O21-C2
45	P	506	3PE	O22-C21-O21-C2
45	Y	201	3PE	O22-C21-O21-C2
45	Y	202	3PE	O22-C21-O21-C2
46	J	202	PC1	O22-C21-O21-C2
46	L	706	PC1	O22-C21-O21-C2
47	A	206	PLC	O'-C'-O2-C2
47	J	205	PLC	O'-C'-O2-C2
47	L	704	PLC	O'-C'-O2-C2
47	d	204	PLC	O'-C'-O2-C2
53	M	602	CDL	OA7-CA5-OA6-CA4
53	N	401	CDL	OA7-CA5-OA6-CA4
53	P	502	CDL	OA7-CA5-OA6-CA4
53	X	201	CDL	OA7-CA5-OA6-CA4
53	i	202	CDL	OA7-CA5-OA6-CA4
45	A	205	3PE	C32-C31-O31-C3
45	J	203	3PE	C32-C31-O31-C3
45	P	504	3PE	C32-C31-O31-C3
45	Y	204	3PE	C32-C31-O31-C3
45	Y	205	3PE	C32-C31-O31-C3
45	Y	206	3PE	C32-C31-O31-C3
46	L	706	PC1	C32-C31-O31-C3
46	L	707	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	d	203	PC1	C32-C31-O31-C3
46	g	202	PC1	C32-C31-O31-C3
46	h	202	PC1	C32-C31-O31-C3
53	M	602	CDL	C71-CB7-OB8-CB6
53	N	401	CDL	C71-CB7-OB8-CB6
53	d	201	CDL	C71-CB7-OB8-CB6
45	A	205	3PE	C22-C21-O21-C2
45	Y	205	3PE	C22-C21-O21-C2
45	a	101	3PE	C22-C21-O21-C2
45	p	201	3PE	C22-C21-O21-C2
45	q	203	3PE	C22-C21-O21-C2
46	B	203	PC1	C22-C21-O21-C2
47	B	202	PLC	C1'-C'-O2-C2
47	L	704	PLC	C1'-C'-O2-C2
53	J	201	CDL	C51-CB5-OB6-CB4
53	i	202	CDL	C51-CB5-OB6-CB4
45	d	202	3PE	O32-C31-O31-C3
49	D	501	U10	C25-C24-C26-C27
49	D	501	U10	C40-C39-C41-C42
49	D	501	U10	C45-C44-C46-C47
49	D	501	U10	C23-C24-C26-C27
49	D	501	U10	C38-C39-C41-C42
45	J	204	3PE	O32-C31-O31-C3
45	Y	208	3PE	C32-C31-O31-C3
45	a	101	3PE	C32-C31-O31-C3
46	H	403	PC1	C32-C31-O31-C3
53	N	401	CDL	C31-CA7-OA8-CA6
45	J	204	3PE	C32-C31-O31-C3
47	h	201	PLC	C1B-CB-O3-C3
46	L	707	PC1	O32-C31-O31-C3
47	d	204	PLC	OB-CB-O3-C3
53	N	401	CDL	OB9-CB7-OB8-CB6
45	L	702	3PE	O22-C21-O21-C2
45	Y	208	3PE	O22-C21-O21-C2
45	j	101	3PE	O22-C21-O21-C2
46	M	604	PC1	O22-C21-O21-C2
53	J	201	CDL	OA7-CA5-OA6-CA4
53	q	201	CDL	OA7-CA5-OA6-CA4
53	d	201	CDL	O1-C1-CA2-OA2
45	d	202	3PE	C32-C31-O31-C3
47	d	204	PLC	C1B-CB-O3-C3
53	J	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
45	Y	208	3PE	O32-C31-O31-C3
45	P	504	3PE	C22-C21-O21-C2
47	P	505	PLC	C1'-C'-O2-C2
53	N	401	CDL	C51-CB5-OB6-CB4
49	D	501	U10	C20-C19-C21-C22
45	a	101	3PE	O32-C31-O31-C3
49	D	501	U10	C14-C16-C17-C18
49	D	501	U10	C34-C36-C37-C38
53	J	201	CDL	OA9-CA7-OA8-CA6
45	A	204	3PE	C32-C31-O31-C3
47	P	505	PLC	O'-C'-O2-C2
53	J	201	CDL	CB2-C1-CA2-OA2
45	P	506	3PE	C32-C31-O31-C3
45	m	202	3PE	C32-C31-O31-C3
46	A	203	PC1	C32-C31-O31-C3
46	I	204	PC1	C32-C31-O31-C3
47	A	206	PLC	C1B-CB-O3-C3
53	d	201	CDL	C31-CA7-OA8-CA6
49	D	501	U10	C43-C44-C46-C47
45	L	702	3PE	C31-C32-C33-C34
45	P	506	3PE	O32-C31-O31-C3
46	I	204	PC1	O32-C31-O31-C3
45	b	101	3PE	C21-C22-C23-C24
45	d	202	3PE	C21-C22-C23-C24
46	P	503	PC1	C31-C32-C33-C34
58	U	101	EHZ	C5-C6-C7-O1
47	A	206	PLC	OB-CB-O3-C3
45	P	504	3PE	O22-C21-O21-C2
53	M	602	CDL	OA5-CA3-CA4-OA6
45	Y	203	3PE	C22-C21-O21-C2
45	J	206	3PE	O21-C2-C3-O31
47	h	201	PLC	OB-CB-O3-C3
45	A	205	3PE	C31-C32-C33-C34
53	M	602	CDL	CA5-C11-C12-C13
45	J	206	3PE	C31-C32-C33-C34
53	N	401	CDL	OB7-CB5-OB6-CB4
49	D	501	U10	C9-C11-C12-C13
45	P	506	3PE	C21-C22-C23-C24
53	J	201	CDL	CB7-C71-C72-C73
46	A	203	PC1	O32-C31-O31-C3
45	J	203	3PE	C22-C21-O21-C2
46	B	203	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
46	B	203	PC1	C31-C32-C33-C34
47	A	206	PLC	C'-C1'-C2'-C3'
53	J	201	CDL	CA5-C11-C12-C13
53	M	602	CDL	CB5-C51-C52-C53
53	M	602	CDL	CB7-C71-C72-C73
53	i	202	CDL	CA5-C11-C12-C13
53	d	201	CDL	OA9-CA7-OA8-CA6
45	A	204	3PE	O32-C31-O31-C3
45	Y	204	3PE	C31-C32-C33-C34
45	g	201	3PE	C31-C32-C33-C34
47	d	204	PLC	C'-C1'-C2'-C3'
45	m	202	3PE	O32-C31-O31-C3
49	D	501	U10	C18-C19-C21-C22
46	H	401	PC1	C31-C32-C33-C34
53	P	502	CDL	CB5-C51-C52-C53
53	P	502	CDL	CB7-C71-C72-C73
46	A	202	PC1	C32-C31-O31-C3
45	J	204	3PE	C22-C21-O21-C2
45	Z	201	3PE	C22-C21-O21-C2
46	P	503	PC1	C22-C21-O21-C2
53	N	401	CDL	CB5-C51-C52-C53
45	Y	201	3PE	C31-C32-C33-C34
53	L	701	CDL	CA5-C11-C12-C13
45	J	203	3PE	O22-C21-O21-C2
45	J	204	3PE	O22-C21-O21-C2
45	Y	203	3PE	O22-C21-O21-C2
45	Z	201	3PE	O22-C21-O21-C2
46	P	503	PC1	O22-C21-O21-C2
45	I	205	3PE	C32-C31-O31-C3
45	J	206	3PE	C32-C31-O31-C3
45	g	201	3PE	C32-C31-O31-C3
46	H	403	PC1	C11-C12-N-C13
46	H	403	PC1	C11-C12-N-C14
53	P	502	CDL	C31-CA7-OA8-CA6
45	H	402	3PE	C22-C21-O21-C2
46	h	202	PC1	C22-C21-O21-C2
46	q	202	PC1	C22-C21-O21-C2
45	H	402	3PE	O22-C21-O21-C2
46	h	202	PC1	O22-C21-O21-C2
53	N	401	CDL	CA7-C31-C32-C33
47	B	202	PLC	C'-C1'-C2'-C3'
45	Y	208	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	C1-C2-O21-C21
53	N	401	CDL	CA6-CA4-OA6-CA5
46	q	202	PC1	O22-C21-O21-C2
46	A	202	PC1	C22-C21-O21-C2
45	m	201	3PE	C31-C32-C33-C34
46	A	202	PC1	O32-C31-O31-C3
45	L	702	3PE	C32-C33-C34-C35
45	Y	204	3PE	C25-C26-C27-C28
46	L	706	PC1	C24-C25-C26-C27
53	d	201	CDL	C72-C73-C74-C75
47	O	403	PLC	C4'-C5'-C6'-C7'
53	M	602	CDL	C14-C15-C16-C17
53	P	502	CDL	C73-C74-C75-C76
45	N	402	3PE	C24-C25-C26-C27
45	H	402	3PE	C23-C24-C25-C26
45	H	402	3PE	C24-C25-C26-C27
45	L	703	3PE	C24-C25-C26-C27
45	M	603	3PE	C28-C29-C2A-C2B
45	N	402	3PE	C2D-C2E-C2F-C2G
45	Y	203	3PE	C3D-C3E-C3F-C3G
45	Y	205	3PE	C29-C2A-C2B-C2C
46	A	203	PC1	C22-C23-C24-C25
46	B	203	PC1	C36-C37-C38-C39
46	B	203	PC1	C3A-C3B-C3C-C3D
46	J	202	PC1	C33-C34-C35-C36
46	L	707	PC1	C38-C39-C3A-C3B
46	L	707	PC1	C3E-C3F-C3G-C3H
53	X	201	CDL	C35-C36-C37-C38
53	d	201	CDL	C41-C42-C43-C44
45	H	402	3PE	C2A-C2B-C2C-C2D
47	d	204	PLC	C5B-C6B-C7B-C8B
46	g	202	PC1	C2D-C2E-C2F-C2G
53	N	401	CDL	C16-C17-C18-C19
53	d	201	CDL	C37-C38-C39-C40
45	m	201	3PE	C22-C21-O21-C2
53	P	502	CDL	C51-CB5-OB6-CB4
45	J	206	3PE	C32-C33-C34-C35
45	Y	206	3PE	C33-C34-C35-C36
47	B	202	PLC	C2B-C3B-C4B-C5B
46	H	401	PC1	C25-C26-C27-C28
46	J	202	PC1	C23-C24-C25-C26
53	M	602	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
53	P	502	CDL	C54-C55-C56-C57
45	P	504	3PE	C21-C22-C23-C24
46	L	706	PC1	C21-C22-C23-C24
45	A	205	3PE	C36-C37-C38-C39
46	A	202	PC1	C32-C33-C34-C35
46	L	707	PC1	C3B-C3C-C3D-C3E
46	q	202	PC1	C28-C29-C2A-C2B
45	I	205	3PE	O32-C31-O31-C3
45	a	101	3PE	C3B-C3C-C3D-C3E
45	d	202	3PE	C26-C27-C28-C29
53	N	401	CDL	C74-C75-C76-C77
45	M	603	3PE	C32-C33-C34-C35
46	H	401	PC1	C27-C28-C29-C2A
45	J	206	3PE	O32-C31-O31-C3
45	g	201	3PE	O32-C31-O31-C3
53	P	502	CDL	OA9-CA7-OA8-CA6
45	J	204	3PE	C29-C2A-C2B-C2C
45	Y	208	3PE	C32-C33-C34-C35
45	g	201	3PE	C34-C35-C36-C37
45	L	705	3PE	C3E-C3F-C3G-C3H
45	m	202	3PE	C3D-C3E-C3F-C3G
46	A	202	PC1	C23-C24-C25-C26
46	L	707	PC1	C39-C3A-C3B-C3C
53	M	602	CDL	C83-C84-C85-C86
53	P	502	CDL	C55-C56-C57-C58
46	M	604	PC1	C1-C2-C3-O31
45	L	705	3PE	C3A-C3B-C3C-C3D
45	P	504	3PE	C32-C33-C34-C35
45	Y	205	3PE	C25-C26-C27-C28
47	B	202	PLC	C5B-C6B-C7B-C8B
53	X	201	CDL	C80-C81-C82-C83
45	M	603	3PE	C3C-C3D-C3E-C3F
45	N	402	3PE	C2A-C2B-C2C-C2D
45	Y	205	3PE	C2B-C2C-C2D-C2E
45	Z	201	3PE	C32-C33-C34-C35
45	g	201	3PE	C3B-C3C-C3D-C3E
53	X	201	CDL	C58-C59-C60-C61
53	d	201	CDL	C35-C36-C37-C38
45	Y	203	3PE	C23-C24-C25-C26
46	h	202	PC1	C27-C28-C29-C2A
45	J	203	3PE	C33-C34-C35-C36
46	I	204	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
46	L	707	PC1	C35-C36-C37-C38
53	X	201	CDL	C63-C64-C65-C66
46	H	403	PC1	C11-C12-N-C15
45	J	204	3PE	C2E-C2F-C2G-C2H
45	g	201	3PE	C3D-C3E-C3F-C3G
53	L	701	CDL	C52-C53-C54-C55
53	N	401	CDL	C71-C72-C73-C74
45	N	402	3PE	C21-C22-C23-C24
45	Y	206	3PE	C31-C32-C33-C34
46	J	202	PC1	C21-C22-C23-C24
45	P	504	3PE	C34-C35-C36-C37
53	P	502	CDL	C60-C61-C62-C63
53	q	201	CDL	C17-C18-C19-C20
45	A	204	3PE	C24-C25-C26-C27
45	j	101	3PE	C31-C32-C33-C34
45	j	101	3PE	C21-C22-C23-C24
45	N	402	3PE	C33-C34-C35-C36
45	Z	201	3PE	C26-C27-C28-C29
45	m	201	3PE	O22-C21-O21-C2
46	A	202	PC1	O22-C21-O21-C2
53	P	502	CDL	OB7-CB5-OB6-CB4
45	b	101	3PE	C35-C36-C37-C38
53	J	201	CDL	C31-C32-C33-C34
45	J	203	3PE	C35-C36-C37-C38
45	Y	203	3PE	C3B-C3C-C3D-C3E
45	Y	203	3PE	C28-C29-C2A-C2B
45	Y	206	3PE	C28-C29-C2A-C2B
45	p	201	3PE	C2D-C2E-C2F-C2G
47	L	704	PLC	C2B-C3B-C4B-C5B
53	P	502	CDL	C76-C77-C78-C79
53	X	201	CDL	C16-C17-C18-C19
53	d	201	CDL	C76-C77-C78-C79
45	L	702	3PE	C21-C22-C23-C24
45	L	703	3PE	C32-C31-O31-C3
46	M	604	PC1	C32-C31-O31-C3
45	b	101	3PE	C36-C37-C38-C39
45	g	201	3PE	C37-C38-C39-C3A
46	I	204	PC1	C22-C23-C24-C25
46	h	202	PC1	C28-C29-C2A-C2B
45	Y	204	3PE	C33-C34-C35-C36
46	A	203	PC1	C23-C24-C25-C26
45	L	702	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
53	J	201	CDL	C73-C74-C75-C76
45	Y	206	3PE	C3A-C3B-C3C-C3D
45	d	202	3PE	C2A-C2B-C2C-C2D
46	H	401	PC1	C32-C33-C34-C35
47	O	403	PLC	C1B-CB-O3-C3
45	L	702	3PE	C23-C24-C25-C26
46	g	202	PC1	C34-C35-C36-C37
53	P	502	CDL	C13-C14-C15-C16
45	A	201	3PE	C22-C21-O21-C2
45	I	205	3PE	C22-C21-O21-C2
46	I	204	PC1	C22-C21-O21-C2
46	L	707	PC1	C22-C21-O21-C2
46	g	202	PC1	C22-C21-O21-C2
47	h	201	PLC	C1'-C'-O2-C2
53	L	701	CDL	C11-CA5-OA6-CA4
46	q	202	PC1	C32-C31-O31-C3
45	d	202	3PE	C31-C32-C33-C34
46	I	204	PC1	O22-C21-O21-C2
46	g	202	PC1	O22-C21-O21-C2
47	h	201	PLC	O'-C'-O2-C2
45	H	402	3PE	C26-C27-C28-C29
45	L	705	3PE	C33-C34-C35-C36
45	Y	203	3PE	C2E-C2F-C2G-C2H
45	Z	201	3PE	C25-C26-C27-C28
46	L	707	PC1	C23-C24-C25-C26
45	d	202	3PE	C34-C35-C36-C37
47	d	204	PLC	C7B-C8B-C9B-CAA
53	L	701	CDL	C14-C15-C16-C17
46	q	202	PC1	C21-C22-C23-C24
45	b	101	3PE	C2C-C2D-C2E-C2F
47	h	201	PLC	C4'-C5'-C6'-C7'
53	X	201	CDL	C12-C13-C14-C15
45	A	201	3PE	C28-C29-C2A-C2B
45	Y	206	3PE	C36-C37-C38-C39
45	Y	208	3PE	C2C-C2D-C2E-C2F
53	i	202	CDL	C57-C58-C59-C60
47	h	201	PLC	C2'-C3'-C4'-C5'
53	N	401	CDL	C72-C73-C74-C75
45	A	201	3PE	C26-C27-C28-C29
53	P	502	CDL	C81-C82-C83-C84
45	Y	204	3PE	C2C-C2D-C2E-C2F
46	h	202	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	P	502	CDL	C53-C54-C55-C56
53	P	502	CDL	C59-C60-C61-C62
53	X	201	CDL	C71-C72-C73-C74
46	L	706	PC1	C31-C32-C33-C34
53	q	201	CDL	CB7-C71-C72-C73
46	M	604	PC1	C23-C24-C25-C26
45	A	201	3PE	O22-C21-O21-C2
46	L	707	PC1	O22-C21-O21-C2
53	L	701	CDL	OA7-CA5-OA6-CA4
46	A	202	PC1	O11-C1-C2-O21
46	A	203	PC1	O11-C1-C2-O21
46	h	202	PC1	O11-C1-C2-O21
47	J	205	PLC	O3P-C1-C2-O2
45	m	202	3PE	C24-C25-C26-C27
45	b	101	3PE	C34-C35-C36-C37
46	H	401	PC1	C36-C37-C38-C39
45	Y	206	3PE	C21-C22-C23-C24
45	Z	201	3PE	O21-C2-C3-O31
46	L	706	PC1	O21-C2-C3-O31
46	M	604	PC1	O21-C2-C3-O31
45	A	205	3PE	C2B-C2C-C2D-C2E
45	p	201	3PE	C2B-C2C-C2D-C2E
47	A	206	PLC	C3'-C4'-C5'-C6'
45	M	603	3PE	C39-C3A-C3B-C3C
47	J	205	PLC	C2B-C3B-C4B-C5B
53	N	401	CDL	C19-C20-C21-C22
53	N	401	CDL	C55-C56-C57-C58
46	h	202	PC1	C33-C34-C35-C36
47	O	403	PLC	C1'-C2'-C3'-C4'
53	X	201	CDL	C52-C53-C54-C55
53	q	201	CDL	C71-C72-C73-C74
45	A	205	3PE	C38-C39-C3A-C3B
45	Y	203	3PE	C22-C23-C24-C25
46	I	203	PC1	C2A-C2B-C2C-C2D
45	N	402	3PE	C35-C36-C37-C38
45	d	202	3PE	C24-C25-C26-C27
53	X	201	CDL	C32-C33-C34-C35
53	d	201	CDL	C31-C32-C33-C34
46	M	604	PC1	C32-C33-C34-C35
53	P	502	CDL	C11-C12-C13-C14
45	J	206	3PE	C27-C28-C29-C2A
45	L	705	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
53	M	602	CDL	C12-C13-C14-C15
53	P	502	CDL	C72-C73-C74-C75
53	M	602	CDL	C39-C40-C41-C42
53	X	201	CDL	C39-C40-C41-C42
53	d	201	CDL	C11-CA5-OA6-CA4
45	Y	203	3PE	C27-C28-C29-C2A
53	L	701	CDL	C39-C40-C41-C42
46	I	204	PC1	C37-C38-C39-C3A
45	L	702	3PE	O11-C1-C2-C3
45	M	603	3PE	O11-C1-C2-C3
45	N	402	3PE	O11-C1-C2-C3
45	Y	208	3PE	O11-C1-C2-C3
46	A	202	PC1	O11-C1-C2-C3
46	h	202	PC1	O11-C1-C2-C3
47	L	704	PLC	O3P-C1-C2-C3
47	d	204	PLC	O3P-C1-C2-C3
53	M	602	CDL	OB5-CB3-CB4-CB6
47	h	201	PLC	C'-C1'-C2'-C3'
45	H	402	3PE	C27-C28-C29-C2A
45	m	202	3PE	C22-C23-C24-C25
53	J	201	CDL	C75-C76-C77-C78
45	L	703	3PE	O32-C31-O31-C3
46	M	604	PC1	O32-C31-O31-C3
45	L	705	3PE	C31-C32-C33-C34
46	H	401	PC1	C21-C22-C23-C24
46	g	202	PC1	C32-C33-C34-C35
46	L	707	PC1	C22-C23-C24-C25
45	b	101	3PE	C2B-C2C-C2D-C2E
53	M	602	CDL	C56-C57-C58-C59
53	M	602	CDL	C62-C63-C64-C65
45	Y	202	3PE	C1-C2-C3-O31
45	Z	201	3PE	C1-C2-C3-O31
46	q	202	PC1	C1-C2-C3-O31
47	A	206	PLC	C1-C2-C3-O3
53	N	401	CDL	CB3-CB4-CB6-OB8
53	d	201	CDL	CA3-CA4-CA6-OA8
53	i	202	CDL	CA3-CA4-CA6-OA8
45	a	101	3PE	C3E-C3F-C3G-C3H
46	H	401	PC1	C37-C38-C39-C3A
46	q	202	PC1	C25-C26-C27-C28
45	A	201	3PE	C22-C23-C24-C25
46	h	202	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
47	Y	207	PLC	C3'-C4'-C5'-C6'
53	M	602	CDL	C34-C35-C36-C37
47	Y	207	PLC	CB-C1B-C2B-C3B
53	N	401	CDL	C34-C35-C36-C37
60	o	201	MYR	C6-C7-C8-C9
45	Y	201	3PE	C32-C33-C34-C35
46	h	202	PC1	C29-C2A-C2B-C2C
46	B	203	PC1	C32-C33-C34-C35
46	q	202	PC1	C2D-C2E-C2F-C2G
53	M	602	CDL	C18-C19-C20-C21
45	j	101	3PE	C1-C2-O21-C21
46	q	202	PC1	C1-C2-O21-C21
53	X	201	CDL	C31-C32-C33-C34
45	L	705	3PE	C25-C26-C27-C28
53	X	201	CDL	C20-C21-C22-C23
46	M	604	PC1	O11-C1-C2-O21
47	P	505	PLC	O3P-C1-C2-O2
53	i	202	CDL	OA5-CA3-CA4-OA6
45	a	101	3PE	C33-C34-C35-C36
45	m	201	3PE	C32-C33-C34-C35
45	L	703	3PE	C36-C37-C38-C39
53	d	201	CDL	C74-C75-C76-C77
57	P	501	NDP	O4D-C1D-N1N-C6N
45	Z	201	3PE	C35-C36-C37-C38
53	q	201	CDL	C13-C14-C15-C16
46	H	401	PC1	C2F-C2G-C2H-C2I
45	a	101	3PE	C36-C37-C38-C39
45	Y	204	3PE	C32-C33-C34-C35
45	Y	208	3PE	C35-C36-C37-C38
45	d	202	3PE	C39-C3A-C3B-C3C
45	j	101	3PE	C27-C28-C29-C2A
47	d	204	PLC	C2'-C3'-C4'-C5'
45	A	205	3PE	O21-C2-C3-O31
45	L	703	3PE	O21-C2-C3-O31
53	J	201	CDL	OA6-CA4-CA6-OA8
45	j	101	3PE	C2B-C2C-C2D-C2E
45	J	204	3PE	C23-C24-C25-C26
47	P	505	PLC	C1'-C2'-C3'-C4'
45	H	402	3PE	C2F-C2G-C2H-C2I
53	X	201	CDL	C44-C45-C46-C47
45	L	705	3PE	C37-C38-C39-C3A
45	J	206	3PE	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
45	b	101	3PE	C3F-C3G-C3H-C3I
53	P	502	CDL	C84-C85-C86-C87
53	q	201	CDL	C31-C32-C33-C34
53	N	401	CDL	CB7-C71-C72-C73
53	d	201	CDL	C11-C12-C13-C14
45	J	206	3PE	C25-C26-C27-C28
60	o	201	MYR	C5-C6-C7-C8
45	M	603	3PE	C22-C23-C24-C25
46	B	203	PC1	C26-C27-C28-C29
49	D	501	U10	C30-C29-C31-C32
53	X	201	CDL	C71-CB7-OB8-CB6
45	g	201	3PE	C3F-C3G-C3H-C3I
53	N	401	CDL	C22-C23-C24-C25
53	q	201	CDL	C14-C15-C16-C17
45	I	205	3PE	O22-C21-O21-C2
45	M	603	3PE	C23-C24-C25-C26
45	Y	208	3PE	C22-C23-C24-C25
53	X	201	CDL	C78-C79-C80-C81
45	P	506	3PE	C2-C1-O11-P
58	T	101	EHZ	S1-C10-C11-N1
45	I	205	3PE	C29-C2A-C2B-C2C
45	Y	206	3PE	C29-C2A-C2B-C2C
46	P	503	PC1	C3C-C3D-C3E-C3F
53	P	502	CDL	C79-C80-C81-C82
45	M	603	3PE	C2B-C2C-C2D-C2E
46	P	503	PC1	C33-C34-C35-C36
45	J	203	3PE	O11-C1-C2-C3
45	Y	205	3PE	O11-C1-C2-C3
45	p	201	3PE	O11-C1-C2-C3
46	A	203	PC1	O11-C1-C2-C3
46	I	204	PC1	O11-C1-C2-C3
46	L	707	PC1	O11-C1-C2-C3
47	J	205	PLC	O3P-C1-C2-C3
47	P	505	PLC	O3P-C1-C2-C3
47	Y	207	PLC	O3P-C1-C2-C3
53	N	401	CDL	OB5-CB3-CB4-CB6
53	d	201	CDL	OA5-CA3-CA4-CA6
53	d	201	CDL	OB5-CB3-CB4-CB6
46	H	403	PC1	C3B-C3C-C3D-C3E
53	X	201	CDL	C54-C55-C56-C57
45	M	603	3PE	C3F-C3G-C3H-C3I
46	H	401	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	Y	205	3PE	C33-C34-C35-C36
46	P	503	PC1	C28-C29-C2A-C2B
53	M	602	CDL	C64-C65-C66-C67
53	J	201	CDL	C37-C38-C39-C40
53	P	502	CDL	C64-C65-C66-C67
46	B	203	PC1	C37-C38-C39-C3A
45	J	203	3PE	C37-C38-C39-C3A
45	A	205	3PE	C25-C26-C27-C28
45	L	703	3PE	C32-C33-C34-C35
53	P	502	CDL	C57-C58-C59-C60
53	N	401	CDL	C78-C79-C80-C81
45	N	402	3PE	C36-C37-C38-C39
46	L	706	PC1	C36-C37-C38-C39
46	h	202	PC1	C37-C38-C39-C3A
46	h	202	PC1	C2A-C2B-C2C-C2D
45	A	205	3PE	C1-C2-C3-O31
45	J	206	3PE	C1-C2-C3-O31
45	b	101	3PE	C1-C2-C3-O31
45	m	202	3PE	C1-C2-C3-O31
46	A	202	PC1	C1-C2-C3-O31
46	H	403	PC1	C1-C2-C3-O31
46	L	706	PC1	C1-C2-C3-O31
46	P	503	PC1	C1-C2-C3-O31
47	J	205	PLC	C1-C2-C3-O3
53	X	201	CDL	CA3-CA4-CA6-OA8
45	I	205	3PE	C23-C24-C25-C26
45	Y	204	3PE	C29-C2A-C2B-C2C
53	L	701	CDL	C36-C37-C38-C39
45	M	603	3PE	C21-C22-C23-C24
58	T	101	EHZ	C4-C5-C6-C7
47	L	704	PLC	C1B-CB-O3-C3
45	m	201	3PE	C27-C28-C29-C2A
45	P	504	3PE	C38-C39-C3A-C3B
53	P	502	CDL	C12-C13-C14-C15
53	X	201	CDL	C84-C85-C86-C87
53	J	201	CDL	CB5-C51-C52-C53
45	g	201	3PE	O11-C1-C2-O21
46	H	401	PC1	O11-C1-C2-O21
47	L	704	PLC	O3P-C1-C2-O2
53	q	201	CDL	OB5-CB3-CB4-OB6
47	A	206	PLC	C4B-C5B-C6B-C7B
58	U	101	EHZ	O3-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C2D-C2E-C2F-C2G
53	X	201	CDL	C61-C62-C63-C64
58	T	101	EHZ	O1-C7-C8-C9
45	Z	201	3PE	C2F-C2G-C2H-C2I
46	h	202	PC1	C26-C27-C28-C29
47	J	205	PLC	C1'-C2'-C3'-C4'
45	I	205	3PE	C26-C27-C28-C29
45	Y	206	3PE	C2D-C2E-C2F-C2G
47	J	205	PLC	C4B-C5B-C6B-C7B
53	P	502	CDL	C62-C63-C64-C65
45	J	204	3PE	O21-C2-C3-O31
45	L	705	3PE	O21-C2-C3-O31
45	P	506	3PE	O21-C2-C3-O31
45	b	101	3PE	O21-C2-C3-O31
46	L	707	PC1	O21-C2-C3-O31
47	J	205	PLC	O2-C2-C3-O3
47	J	205	PLC	C8B-C9B-CAA-CBA
53	d	201	CDL	OA7-CA5-OA6-CA4
53	J	201	CDL	C53-C54-C55-C56
46	A	203	PC1	C24-C25-C26-C27
46	L	707	PC1	C21-C22-C23-C24
45	A	201	3PE	C32-C33-C34-C35
45	A	201	3PE	C36-C37-C38-C39
45	Y	208	3PE	C3B-C3C-C3D-C3E
60	o	201	MYR	C4-C5-C6-C7
45	Y	203	3PE	C38-C39-C3A-C3B
47	O	403	PLC	OB-CB-O3-C3
49	D	501	U10	C29-C31-C32-C33
53	X	201	CDL	C32-C31-CA7-OA8
45	L	702	3PE	C3D-C3E-C3F-C3G
45	I	205	3PE	C25-C26-C27-C28
53	d	201	CDL	CB2-C1-CA2-OA2
45	A	201	3PE	C33-C34-C35-C36
45	I	205	3PE	C2C-C2D-C2E-C2F
47	A	206	PLC	C6'-C7'-C8'-C9'
45	L	703	3PE	O11-C1-C2-C3
45	Y	204	3PE	O11-C1-C2-C3
45	g	201	3PE	O11-C1-C2-C3
45	m	201	3PE	O11-C1-C2-C3
46	J	202	PC1	O11-C1-C2-C3
53	M	602	CDL	OA5-CA3-CA4-CA6
45	J	203	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
53	M	602	CDL	C11-C12-C13-C14
46	I	203	PC1	C22-C23-C24-C25
46	I	203	PC1	C34-C35-C36-C37
45	b	101	3PE	C32-C33-C34-C35
45	Y	206	3PE	C2C-C2D-C2E-C2F
47	L	704	PLC	OB-CB-O3-C3
45	g	201	3PE	C39-C3A-C3B-C3C
53	J	201	CDL	C38-C39-C40-C41
46	h	202	PC1	C32-C33-C34-C35
53	P	502	CDL	C14-C15-C16-C17
53	X	201	CDL	OB9-CB7-OB8-CB6
47	h	201	PLC	C1'-C2'-C3'-C4'
53	X	201	CDL	CA5-C11-C12-C13
46	q	202	PC1	O32-C31-O31-C3
45	Y	203	3PE	C34-C35-C36-C37
45	A	205	3PE	C23-C24-C25-C26
45	Y	204	3PE	C3-C2-O21-C21
45	Y	208	3PE	C3-C2-O21-C21
46	I	204	PC1	C38-C39-C3A-C3B
46	I	204	PC1	C24-C25-C26-C27
45	P	506	3PE	C27-C28-C29-C2A
45	Y	201	3PE	C36-C37-C38-C39
45	J	206	3PE	C39-C3A-C3B-C3C
45	Y	206	3PE	C2B-C2C-C2D-C2E
45	J	203	3PE	O11-C1-C2-O21
45	Y	206	3PE	O11-C1-C2-O21
45	m	201	3PE	O11-C1-C2-O21
45	p	201	3PE	O11-C1-C2-O21
45	q	203	3PE	O11-C1-C2-O21
46	L	707	PC1	O11-C1-C2-O21
46	P	503	PC1	O11-C1-C2-O21
47	Y	207	PLC	O3P-C1-C2-O2
47	h	201	PLC	O3P-C1-C2-O2
53	X	201	CDL	OB5-CB3-CB4-OB6
45	P	506	3PE	C25-C26-C27-C28
45	A	204	3PE	C1-C2-C3-O31
46	L	707	PC1	C1-C2-C3-O31
46	d	203	PC1	C1-C2-C3-O31
46	g	202	PC1	C1-C2-C3-O31
49	D	501	U10	C24-C26-C27-C28
45	m	201	3PE	C33-C34-C35-C36
53	M	602	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
45	J	203	3PE	C12-C11-O13-P
45	J	204	3PE	C12-C11-O13-P
45	L	703	3PE	C12-C11-O13-P
45	Y	201	3PE	C12-C11-O13-P
45	Y	208	3PE	C12-C11-O13-P
45	Z	201	3PE	C12-C11-O13-P
45	a	101	3PE	C12-C11-O13-P
45	b	101	3PE	C12-C11-O13-P
45	j	101	3PE	C12-C11-O13-P
45	m	201	3PE	C12-C11-O13-P
45	p	201	3PE	C12-C11-O13-P
47	J	205	PLC	C5-C4-O4P-P
47	L	704	PLC	C5-C4-O4P-P
53	J	201	CDL	C51-C52-C53-C54
45	L	702	3PE	O21-C2-C3-O31
45	P	504	3PE	O21-C2-C3-O31
45	Y	202	3PE	O21-C2-C3-O31
45	Y	203	3PE	O21-C2-C3-O31
45	m	202	3PE	O21-C2-C3-O31
46	A	202	PC1	O21-C2-C3-O31
46	H	403	PC1	O21-C2-C3-O31
46	d	203	PC1	O21-C2-C3-O31
46	g	202	PC1	O21-C2-C3-O31
53	X	201	CDL	OA6-CA4-CA6-OA8
53	d	201	CDL	OA6-CA4-CA6-OA8
46	g	202	PC1	C2A-C2B-C2C-C2D
47	Y	207	PLC	C6'-C7'-C8'-C9'
53	M	602	CDL	C37-C38-C39-C40
45	N	402	3PE	C23-C24-C25-C26
53	L	701	CDL	C55-C56-C57-C58
53	L	701	CDL	CB5-C51-C52-C53
45	Y	204	3PE	C37-C38-C39-C3A
53	M	602	CDL	C40-C41-C42-C43
53	M	602	CDL	C42-C43-C44-C45
45	Y	205	3PE	C27-C28-C29-C2A
45	p	201	3PE	C23-C24-C25-C26
45	Y	208	3PE	C38-C39-C3A-C3B
53	N	401	CDL	C76-C77-C78-C79
45	P	506	3PE	C28-C29-C2A-C2B
46	q	202	PC1	O13-C11-C12-N
47	A	206	PLC	O4P-C4-C5-N
47	B	202	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
45	L	702	3PE	C25-C26-C27-C28
49	D	501	U10	C12-C11-C9-C10
46	h	202	PC1	C2F-C2G-C2H-C2I
45	N	402	3PE	C2F-C2G-C2H-C2I
46	L	707	PC1	C33-C34-C35-C36
53	N	401	CDL	C17-C18-C19-C20
53	q	201	CDL	C31-CA7-OA8-CA6
46	d	203	PC1	C3B-C3C-C3D-C3E
58	T	101	EHZ	C2-C3-C4-C5
45	p	201	3PE	C26-C27-C28-C29
53	X	201	CDL	CA7-C31-C32-C33
45	Y	203	3PE	C39-C3A-C3B-C3C
53	X	201	CDL	C33-C34-C35-C36
45	Y	206	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
46	M	604	PC1	O11-C1-C2-C3
47	h	201	PLC	O3P-C1-C2-C3
53	i	202	CDL	OA5-CA3-CA4-CA6
58	U	101	EHZ	C1-C21-C22-C23
45	Y	204	3PE	O22-C21-O21-C2
53	q	201	CDL	OB7-CB5-OB6-CB4
45	j	101	3PE	C33-C34-C35-C36
58	T	101	EHZ	C18-C17-C20-O6
45	J	204	3PE	C2C-C2D-C2E-C2F
45	Y	205	3PE	C2E-C2F-C2G-C2H
45	m	201	3PE	C2B-C2C-C2D-C2E
45	J	204	3PE	C25-C26-C27-C28
58	U	101	EHZ	C3-C4-C5-C6
53	q	201	CDL	OA9-CA7-OA8-CA6
53	d	201	CDL	C1-CB2-OB2-PB2
45	L	702	3PE	O11-C1-C2-O21
45	Y	208	3PE	O11-C1-C2-O21
46	J	202	PC1	O11-C1-C2-O21
46	L	706	PC1	O11-C1-C2-O21
47	B	202	PLC	O3P-C1-C2-O2
53	N	401	CDL	OB5-CB3-CB4-OB6
53	d	201	CDL	OA5-CA3-CA4-OA6
53	d	201	CDL	OB5-CB3-CB4-OB6
45	Y	204	3PE	C22-C21-O21-C2
53	q	201	CDL	C51-CB5-OB6-CB4
58	U	101	EHZ	C21-C1-C2-C3
45	Y	204	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
45	j	101	3PE	C35-C36-C37-C38
45	H	402	3PE	C32-C33-C34-C35
46	H	403	PC1	C3E-C3F-C3G-C3H
47	h	201	PLC	C7'-C8'-C9'-CA'
53	L	701	CDL	C59-C60-C61-C62
53	M	602	CDL	C59-C60-C61-C62
45	A	205	3PE	C24-C25-C26-C27
45	p	201	3PE	C27-C28-C29-C2A
45	a	101	3PE	O21-C2-C3-O31
46	P	503	PC1	O21-C2-C3-O31
47	A	206	PLC	O2-C2-C3-O3
47	P	505	PLC	O2-C2-C3-O3
53	J	201	CDL	OB6-CB4-CB6-OB8
53	q	201	CDL	OA6-CA4-CA6-OA8
45	H	402	3PE	C1-C2-C3-O31
45	J	204	3PE	C1-C2-C3-O31
45	L	702	3PE	C1-C2-C3-O31
45	L	705	3PE	C1-C2-C3-O31
45	P	506	3PE	C1-C2-C3-O31
45	Y	203	3PE	C1-C2-C3-O31
47	P	505	PLC	C1-C2-C3-O3
53	J	201	CDL	CB3-CB4-CB6-OB8
53	q	201	CDL	CA3-CA4-CA6-OA8
45	a	101	3PE	C3A-C3B-C3C-C3D
60	o	201	MYR	C10-C11-C12-C13
58	T	101	EHZ	C16-C17-C20-O6
53	L	701	CDL	C13-C14-C15-C16
45	A	201	3PE	C3B-C3C-C3D-C3E
45	b	101	3PE	C3C-C3D-C3E-C3F
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C11-O13-P-O14
45	A	204	3PE	O13-C11-C12-N
45	I	205	3PE	C11-O13-P-O11
45	I	205	3PE	C11-O13-P-O12
45	I	205	3PE	C11-O13-P-O14
45	J	203	3PE	C1-O11-P-O14
45	J	206	3PE	C1-O11-P-O14
45	L	703	3PE	C1-O11-P-O14
45	L	705	3PE	C1-O11-P-O14
45	M	603	3PE	O13-C11-C12-N
45	N	402	3PE	C11-O13-P-O14
45	P	504	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	P	504	3PE	C11-O13-P-O12
45	P	504	3PE	C11-O13-P-O14
45	Y	201	3PE	C1-O11-P-O14
45	Y	202	3PE	O13-C11-C12-N
45	Y	204	3PE	C1-O11-P-O14
45	Y	205	3PE	C1-O11-P-O13
45	Y	205	3PE	C1-O11-P-O14
45	Y	205	3PE	C11-O13-P-O11
45	Y	206	3PE	C1-O11-P-O14
45	Y	206	3PE	C11-O13-P-O11
45	Y	206	3PE	C11-O13-P-O12
45	Y	206	3PE	C11-O13-P-O14
45	Y	206	3PE	O13-C11-C12-N
45	Z	201	3PE	C1-O11-P-O12
45	Z	201	3PE	C1-O11-P-O13
45	Z	201	3PE	C1-O11-P-O14
45	Z	201	3PE	C11-O13-P-O14
45	b	101	3PE	C1-O11-P-O14
45	g	201	3PE	C11-O13-P-O14
45	m	201	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O12
45	m	201	3PE	C11-O13-P-O14
45	m	202	3PE	C1-O11-P-O12
45	m	202	3PE	C11-O13-P-O11
45	m	202	3PE	C11-O13-P-O12
45	m	202	3PE	C11-O13-P-O14
45	p	201	3PE	C1-O11-P-O13
46	A	202	PC1	C1-O11-P-O12
46	H	403	PC1	C11-O13-P-O14
46	I	203	PC1	C11-O13-P-O14
46	I	203	PC1	C11-O13-P-O11
46	I	204	PC1	C11-O13-P-O11
46	J	202	PC1	C11-O13-P-O14
46	L	707	PC1	C11-O13-P-O14
46	g	202	PC1	C11-O13-P-O12
46	g	202	PC1	C11-O13-P-O14
46	g	202	PC1	C11-O13-P-O11
46	h	202	PC1	C1-O11-P-O14
46	h	202	PC1	C1-O11-P-O13
47	A	206	PLC	C4-O4P-P-O1P
47	L	704	PLC	C1-O3P-P-O4P
47	O	403	PLC	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
47	P	505	PLC	C4-O4P-P-O2P
53	J	201	CDL	CA3-OA5-PA1-OA3
53	L	701	CDL	CA2-OA2-PA1-OA3
53	L	701	CDL	CA2-OA2-PA1-OA4
53	L	701	CDL	CA2-OA2-PA1-OA5
53	L	701	CDL	CA3-OA5-PA1-OA4
53	M	602	CDL	CB3-OB5-PB2-OB3
53	N	401	CDL	CA2-OA2-PA1-OA4
53	N	401	CDL	CA3-OA5-PA1-OA2
53	N	401	CDL	CA3-OA5-PA1-OA3
53	N	401	CDL	CA3-OA5-PA1-OA4
53	N	401	CDL	CB2-OB2-PB2-OB3
53	N	401	CDL	CB2-OB2-PB2-OB4
53	N	401	CDL	CB2-OB2-PB2-OB5
53	P	502	CDL	CB2-OB2-PB2-OB3
53	X	201	CDL	CA2-OA2-PA1-OA3
53	X	201	CDL	CB2-OB2-PB2-OB3
53	q	201	CDL	CA3-OA5-PA1-OA3
53	q	201	CDL	CB2-OB2-PB2-OB3
45	q	203	3PE	O21-C21-C22-C23
45	L	702	3PE	C39-C3A-C3B-C3C
49	D	501	U10	C12-C11-C9-C8
45	L	705	3PE	C34-C35-C36-C37
46	A	203	PC1	C2-C1-O11-P
46	B	203	PC1	C2-C1-O11-P
47	d	204	PLC	C2-C1-O3P-P
51	F	501	FMN	C4'-C5'-O5'-P
53	N	401	CDL	C24-C25-C26-C27
45	I	205	3PE	C21-C22-C23-C24
45	m	202	3PE	C35-C36-C37-C38
49	D	501	U10	C11-C12-C13-C14
59	i	201	CHD	C13-C17-C20-C21
53	X	201	CDL	C77-C78-C79-C80
47	O	403	PLC	C8'-C9'-CA'-CB'
53	i	202	CDL	C51-C52-C53-C54
45	L	702	3PE	C3-C2-O21-C21
45	L	705	3PE	C1-C2-O21-C21
45	b	101	3PE	C3-C2-O21-C21
45	Y	203	3PE	C36-C37-C38-C39
45	m	201	3PE	C2A-C2B-C2C-C2D
45	q	203	3PE	O11-C1-C2-C3
47	B	202	PLC	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
53	q	201	CDL	OB5-CB3-CB4-CB6
45	Y	203	3PE	C29-C2A-C2B-C2C
45	m	202	3PE	C3C-C3D-C3E-C3F
45	Y	201	3PE	C21-C22-C23-C24
45	Y	204	3PE	O11-C1-C2-O21
53	i	202	CDL	C71-C72-C73-C74
45	b	101	3PE	C2F-C2G-C2H-C2I
49	D	501	U10	C36-C37-C38-C39
53	i	202	CDL	OA6-CA4-CA6-OA8
45	m	202	3PE	C25-C26-C27-C28
45	j	101	3PE	C29-C2A-C2B-C2C
46	A	203	PC1	C32-C33-C34-C35
46	I	203	PC1	C2C-C2D-C2E-C2F
53	N	401	CDL	C56-C57-C58-C59
45	Y	206	3PE	C2A-C2B-C2C-C2D
47	J	205	PLC	C4'-C5'-C6'-C7'
45	L	703	3PE	C1-C2-C3-O31
53	J	201	CDL	CA3-CA4-CA6-OA8
45	b	101	3PE	C3E-C3F-C3G-C3H
55	O	401	DGT	PA-O3A-PB-O1B
53	L	701	CDL	C32-C31-CA7-OA8
45	q	203	3PE	O22-C21-C22-C23
45	L	705	3PE	C23-C24-C25-C26
45	Y	204	3PE	C36-C37-C38-C39
53	N	401	CDL	CA5-C11-C12-C13
45	N	402	3PE	O32-C31-O31-C3
45	p	201	3PE	C2A-C2B-C2C-C2D
45	I	205	3PE	C32-C33-C34-C35
46	d	203	PC1	C11-C12-N-C15
57	P	501	NDP	C2B-O2B-P2B-O2X
53	i	202	CDL	C14-C15-C16-C17
45	N	402	3PE	C32-C31-O31-C3
47	B	202	PLC	C1B-CB-O3-C3
46	M	604	PC1	C2-C1-O11-P
45	Z	201	3PE	C2A-C2B-C2C-C2D
53	X	201	CDL	C82-C83-C84-C85
45	b	101	3PE	C32-C31-O31-C3
45	P	506	3PE	O11-C1-C2-O21
45	a	101	3PE	O11-C1-C2-O21
53	P	502	CDL	OB5-CB3-CB4-OB6
53	i	202	CDL	OB5-CB3-CB4-OB6
46	I	204	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
47	B	202	PLC	OB-CB-O3-C3
53	X	201	CDL	C36-C37-C38-C39
45	A	205	3PE	C2C-C2D-C2E-C2F
45	A	205	3PE	C35-C36-C37-C38
45	b	101	3PE	C38-C39-C3A-C3B
45	b	101	3PE	C3B-C3C-C3D-C3E
45	J	204	3PE	C27-C28-C29-C2A
45	Y	203	3PE	C35-C36-C37-C38
46	P	503	PC1	C23-C24-C25-C26
45	L	702	3PE	C38-C39-C3A-C3B
46	H	401	PC1	C2D-C2E-C2F-C2G
45	b	101	3PE	O32-C31-O31-C3
46	d	203	PC1	C35-C36-C37-C38
47	Y	207	PLC	C8'-C9'-CA'-CB'
45	N	402	3PE	C22-C23-C24-C25
53	i	202	CDL	C13-C14-C15-C16
45	N	402	3PE	C3C-C3D-C3E-C3F
46	P	503	PC1	C25-C26-C27-C28
45	L	703	3PE	C25-C26-C27-C28
46	A	202	PC1	C26-C27-C28-C29
46	H	401	PC1	C33-C34-C35-C36
46	P	503	PC1	C38-C39-C3A-C3B
46	I	203	PC1	C32-C33-C34-C35
45	L	702	3PE	C27-C28-C29-C2A
45	a	101	3PE	C37-C38-C39-C3A
45	p	201	3PE	C22-C23-C24-C25
45	J	203	3PE	C2-C1-O11-P
53	M	602	CDL	C81-C82-C83-C84
58	U	101	EHZ	N1-C12-C13-C14
53	N	401	CDL	C32-C33-C34-C35
46	g	202	PC1	C23-C24-C25-C26
45	A	201	3PE	C2A-C2B-C2C-C2D
45	N	402	3PE	C3A-C3B-C3C-C3D
45	Z	201	3PE	C2D-C2E-C2F-C2G
46	H	401	PC1	C34-C35-C36-C37
45	J	206	3PE	C38-C39-C3A-C3B
46	H	401	PC1	C23-C24-C25-C26
45	a	101	3PE	C1-C2-C3-O31
45	I	205	3PE	C27-C28-C29-C2A
46	d	203	PC1	C23-C24-C25-C26
46	h	202	PC1	C2B-C2C-C2D-C2E
45	L	703	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
45	P	506	3PE	C3-C2-O21-C21
47	P	505	PLC	C3-C2-O2-C'
47	Y	207	PLC	C1-C2-O2-C'
53	X	201	CDL	CA3-CA4-OA6-CA5
53	X	201	CDL	CA6-CA4-OA6-CA5
45	g	201	3PE	C38-C39-C3A-C3B
53	N	401	CDL	C35-C36-C37-C38
45	g	201	3PE	C22-C23-C24-C25
53	N	401	CDL	C57-C58-C59-C60
53	X	201	CDL	C75-C76-C77-C78
53	q	201	CDL	C52-C51-CB5-OB6
46	I	203	PC1	C31-C32-C33-C34
46	H	401	PC1	O22-C21-C22-C23
59	i	201	CHD	C22-C23-C24-O25
46	A	203	PC1	C21-C22-C23-C24
45	Y	201	3PE	C22-C23-C24-C25
45	j	101	3PE	C38-C39-C3A-C3B
45	Y	208	3PE	C39-C3A-C3B-C3C
45	L	703	3PE	C21-C22-C23-C24
45	Y	203	3PE	C21-C22-C23-C24
45	H	402	3PE	C2-C1-O11-P
45	L	702	3PE	C2-C1-O11-P
47	A	206	PLC	C2-C1-O3P-P
45	Y	203	3PE	C2F-C2G-C2H-C2I
46	g	202	PC1	C2F-C2G-C2H-C2I
46	H	401	PC1	O11-C1-C2-C3
53	q	201	CDL	C12-C13-C14-C15
49	D	501	U10	C49-C51-C52-C53
45	H	402	3PE	C2C-C2D-C2E-C2F
46	B	203	PC1	C22-C23-C24-C25
45	H	402	3PE	C2D-C2E-C2F-C2G
45	b	101	3PE	C3D-C3E-C3F-C3G
47	d	204	PLC	C2B-C3B-C4B-C5B
45	A	205	3PE	C32-C33-C34-C35
45	M	603	3PE	C3B-C3C-C3D-C3E
46	I	203	PC1	C2D-C2E-C2F-C2G
46	H	401	PC1	C11-C12-N-C13
46	H	401	PC1	C11-C12-N-C15
46	d	203	PC1	C11-C12-N-C14
45	m	202	3PE	C38-C39-C3A-C3B
45	A	205	3PE	C21-C22-C23-C24
46	h	202	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
59	i	201	CHD	C22-C23-C24-O26
49	D	501	U10	C28-C29-C31-C32
53	N	401	CDL	C11-C12-C13-C14
45	Y	205	3PE	C21-C22-C23-C24
53	i	202	CDL	C73-C74-C75-C76
53	i	202	CDL	O1-C1-CB2-OB2
45	Y	208	3PE	C3F-C3G-C3H-C3I
46	H	403	PC1	C3F-C3G-C3H-C3I
45	Y	204	3PE	C27-C28-C29-C2A
46	L	706	PC1	C3D-C3E-C3F-C3G
53	d	201	CDL	C75-C76-C77-C78
45	L	703	3PE	C35-C36-C37-C38
53	M	602	CDL	C80-C81-C82-C83
49	D	501	U10	C50-C49-C51-C52
53	N	401	CDL	CA4-CA3-OA5-PA1
53	P	502	CDL	C1-CB2-OB2-PB2
45	A	205	3PE	C33-C34-C35-C36
46	L	706	PC1	C38-C39-C3A-C3B
45	L	705	3PE	C27-C28-C29-C2A
53	X	201	CDL	CB3-CB4-CB6-OB8
45	N	402	3PE	C37-C38-C39-C3A
46	P	503	PC1	C22-C23-C24-C25
45	Y	206	3PE	O22-C21-O21-C2
49	D	501	U10	C35-C34-C36-C37
53	M	602	CDL	C72-C73-C74-C75
45	A	201	3PE	O21-C21-C22-C23
45	H	402	3PE	O21-C21-C22-C23
53	M	602	CDL	C13-C14-C15-C16
46	H	401	PC1	C11-C12-N-C14
45	J	203	3PE	C39-C3A-C3B-C3C
45	L	703	3PE	O31-C31-C32-C33
45	Y	203	3PE	C33-C34-C35-C36
53	M	602	CDL	C53-C54-C55-C56
53	i	202	CDL	C75-C76-C77-C78
46	L	706	PC1	O11-C1-C2-C3
46	P	503	PC1	O11-C1-C2-C3
53	X	201	CDL	OB5-CB3-CB4-CB6
53	i	202	CDL	OB5-CB3-CB4-CB6
45	q	203	3PE	O31-C31-C32-C33
45	M	603	3PE	C35-C36-C37-C38
53	X	201	CDL	C19-C20-C21-C22
46	I	204	PC1	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
53	X	201	CDL	O1-C1-CA2-OA2
45	Y	204	3PE	C2A-C2B-C2C-C2D
57	P	501	NDP	O4B-C4B-C5B-O5B
53	M	602	CDL	C36-C37-C38-C39
51	F	501	FMN	C5'-O5'-P-O2P
45	P	506	3PE	C24-C25-C26-C27
45	j	101	3PE	C37-C38-C39-C3A
45	m	202	3PE	C26-C27-C28-C29
46	L	707	PC1	C24-C25-C26-C27
45	m	201	3PE	O21-C21-C22-C23
53	L	701	CDL	C33-C34-C35-C36
45	A	205	3PE	C2A-C2B-C2C-C2D
45	P	506	3PE	C1-C2-O21-C21
55	O	401	DGT	PB-O3B-PG-O2G
46	P	503	PC1	C32-C33-C34-C35
46	I	204	PC1	C3B-C3C-C3D-C3E
53	M	602	CDL	C82-C83-C84-C85
46	L	706	PC1	C39-C3A-C3B-C3C
53	L	701	CDL	O1-C1-CA2-OA2
46	H	403	PC1	C35-C36-C37-C38
53	L	701	CDL	C64-C65-C66-C67
53	L	701	CDL	C62-C63-C64-C65
53	M	602	CDL	C78-C79-C80-C81
53	M	602	CDL	C12-C11-CA5-OA6
53	P	502	CDL	OA5-CA3-CA4-OA6
46	d	203	PC1	C11-C12-N-C13
53	J	201	CDL	C35-C36-C37-C38
45	P	504	3PE	C1-C2-C3-O31
53	M	602	CDL	CB3-CB4-CB6-OB8
58	U	101	EHZ	C21-C22-C23-C24
45	a	101	3PE	C38-C39-C3A-C3B
45	m	201	3PE	C25-C26-C27-C28
46	I	204	PC1	C29-C2A-C2B-C2C
45	A	204	3PE	O31-C31-C32-C33
53	N	401	CDL	C52-C51-CB5-OB6
46	H	401	PC1	C35-C36-C37-C38
45	q	203	3PE	C12-C11-O13-P
46	g	202	PC1	C2B-C2C-C2D-C2E
46	L	706	PC1	C32-C33-C34-C35
47	J	205	PLC	C5B-C6B-C7B-C8B
53	X	201	CDL	C74-C75-C76-C77
45	J	206	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
46	g	202	PC1	C29-C2A-C2B-C2C
53	M	602	CDL	OB6-CB4-CB6-OB8
45	Y	208	3PE	C33-C34-C35-C36
46	L	707	PC1	C26-C27-C28-C29
53	L	701	CDL	C57-C58-C59-C60
45	A	204	3PE	O21-C21-C22-C23
46	H	403	PC1	C32-C33-C34-C35
45	a	101	3PE	O11-C1-C2-C3
53	q	201	CDL	C19-C20-C21-C22
53	X	201	CDL	C32-C31-CA7-OA9
45	a	101	3PE	O21-C21-C22-C23
45	Y	203	3PE	O31-C31-C32-C33
46	I	203	PC1	O22-C21-O21-C2
46	H	403	PC1	C39-C3A-C3B-C3C
53	N	401	CDL	C20-C21-C22-C23
45	g	201	3PE	C35-C36-C37-C38
46	I	204	PC1	O13-C11-C12-N
46	h	202	PC1	O13-C11-C12-N
55	O	401	DGT	PB-O3A-PA-O1A
55	O	401	DGT	PB-O3A-PA-O2A
46	B	203	PC1	C3B-C3C-C3D-C3E
47	J	205	PLC	C2B-C1B-CB-O3
53	J	201	CDL	C52-C51-CB5-OB6
45	Y	206	3PE	C22-C21-O21-C2
53	J	201	CDL	CA7-C31-C32-C33
45	N	402	3PE	C38-C39-C3A-C3B
45	Y	201	3PE	O21-C21-C22-C23
45	A	201	3PE	C29-C2A-C2B-C2C
53	i	202	CDL	C39-C40-C41-C42
45	j	101	3PE	O21-C21-C22-C23
47	L	704	PLC	O2-C'-C1'-C2'
46	q	202	PC1	O11-C1-C2-O21
47	A	206	PLC	O3P-C1-C2-O2
58	T	101	EHZ	O4-C15-C16-C17
45	Y	202	3PE	O31-C31-C32-C33
45	Y	206	3PE	O31-C31-C32-C33
53	d	201	CDL	C72-C71-CB7-OB8
53	N	401	CDL	C18-C19-C20-C21
45	Y	201	3PE	C38-C39-C3A-C3B
53	i	202	CDL	C74-C75-C76-C77
53	J	201	CDL	C72-C71-CB7-OB8
53	X	201	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
46	H	401	PC1	O22-C21-O21-C2
45	Y	201	3PE	C28-C29-C2A-C2B
45	L	703	3PE	O21-C21-C22-C23
46	I	203	PC1	O31-C31-C32-C33
53	J	201	CDL	C12-C11-CA5-OA6
53	M	602	CDL	C63-C64-C65-C66
45	A	201	3PE	C2C-C2D-C2E-C2F
46	I	203	PC1	C22-C21-O21-C2
46	g	202	PC1	O21-C21-C22-C23
53	L	701	CDL	C52-C51-CB5-OB6
46	L	706	PC1	C35-C36-C37-C38
45	J	206	3PE	C37-C38-C39-C3A
45	H	402	3PE	O31-C31-C32-C33
45	M	603	3PE	O21-C21-C22-C23
45	Y	201	3PE	O31-C31-C32-C33
45	g	201	3PE	O21-C21-C22-C23
46	L	707	PC1	O21-C21-C22-C23
47	d	204	PLC	C2B-C1B-CB-O3
55	O	401	DGT	PB-O3B-PG-O3G
53	M	602	CDL	C73-C74-C75-C76
45	A	205	3PE	O21-C21-C22-C23
46	I	203	PC1	C2B-C2C-C2D-C2E
53	q	201	CDL	C53-C54-C55-C56
45	Y	208	3PE	C3E-C3F-C3G-C3H
51	F	501	FMN	N10-C1'-C2'-O2'
58	T	101	EHZ	C19-C17-C20-O6
46	q	202	PC1	C26-C27-C28-C29
45	A	201	3PE	O31-C31-C32-C33
45	J	203	3PE	C38-C39-C3A-C3B
45	a	101	3PE	C39-C3A-C3B-C3C
47	Y	207	PLC	C'-C1'-C2'-C3'
60	o	201	MYR	C7-C8-C9-C10
46	I	204	PC1	C11-C12-N-C15
46	L	707	PC1	C11-C12-N-C14
46	H	403	PC1	C36-C37-C38-C39
58	T	101	EHZ	N2-C15-C16-C17
51	F	501	FMN	O3'-C3'-C4'-C5'
45	N	402	3PE	C29-C2A-C2B-C2C
46	L	707	PC1	C37-C38-C39-C3A
45	N	402	3PE	C2-C1-O11-P
45	P	504	3PE	C2-C1-O11-P
45	Z	201	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
45	A	205	3PE	C26-C27-C28-C29
45	d	202	3PE	C3A-C3B-C3C-C3D
47	J	205	PLC	C2B-C1B-CB-OB
47	L	704	PLC	O'-C'-C1'-C2'
47	J	205	PLC	OB-CB-O3-C3
47	J	205	PLC	C1B-CB-O3-C3
45	Y	205	3PE	C26-C27-C28-C29
46	H	403	PC1	C33-C34-C35-C36
45	Y	205	3PE	O21-C21-C22-C23
45	P	506	3PE	C33-C34-C35-C36
46	I	204	PC1	C11-C12-N-C13
45	Y	201	3PE	O32-C31-C32-C33
45	j	101	3PE	O22-C21-C22-C23
53	J	201	CDL	C72-C71-CB7-OB9
45	A	205	3PE	C3E-C3F-C3G-C3H
45	A	205	3PE	C22-C23-C24-C25
46	H	403	PC1	C34-C35-C36-C37
45	A	204	3PE	O32-C31-C32-C33
45	Y	202	3PE	O32-C31-C32-C33
45	Y	203	3PE	O32-C31-C32-C33
45	Y	201	3PE	C35-C36-C37-C38
45	Y	208	3PE	C34-C35-C36-C37
57	P	501	NDP	C3B-C4B-C5B-O5B
46	H	401	PC1	C22-C21-O21-C2
45	A	204	3PE	O22-C21-C22-C23
45	A	205	3PE	O22-C21-C22-C23
45	L	703	3PE	O22-C21-C22-C23
45	g	201	3PE	O22-C21-C22-C23
46	I	203	PC1	O32-C31-C32-C33
45	H	402	3PE	O21-C2-C3-O31
46	h	202	PC1	C2D-C2E-C2F-C2G
53	N	401	CDL	C52-C51-CB5-OB7
53	P	502	CDL	C72-C71-CB7-OB8
45	Y	204	3PE	C38-C39-C3A-C3B
46	g	202	PC1	O22-C21-C22-C23
53	i	202	CDL	C1-CA2-OA2-PA1
45	H	402	3PE	C35-C36-C37-C38
46	I	204	PC1	C11-C12-N-C14
46	L	707	PC1	C11-C12-N-C13
46	L	707	PC1	C11-C12-N-C15
46	P	503	PC1	C11-C12-N-C14
45	M	603	3PE	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	O22-C21-C22-C23
53	J	201	CDL	C52-C51-CB5-OB7
45	Y	206	3PE	C2F-C2G-C2H-C2I
53	d	201	CDL	C72-C71-CB7-OB9
53	P	502	CDL	C77-C78-C79-C80
45	Y	206	3PE	O32-C31-C32-C33
45	N	402	3PE	O21-C21-C22-C23
45	L	702	3PE	C3B-C3C-C3D-C3E
53	d	201	CDL	C42-C43-C44-C45
45	Y	201	3PE	C26-C27-C28-C29
45	J	206	3PE	O21-C21-C22-C23
53	X	201	CDL	C52-C51-CB5-OB6
57	P	501	NDP	PA-O3-PN-O2N
45	A	201	3PE	O32-C31-C32-C33
45	H	402	3PE	O32-C31-C32-C33
46	L	707	PC1	O22-C21-C22-C23
47	d	204	PLC	C2B-C1B-CB-OB
45	J	204	3PE	C2D-C2E-C2F-C2G
53	i	202	CDL	C72-C73-C74-C75

There are no ring outliers.

29 monomers are involved in 55 short contacts:

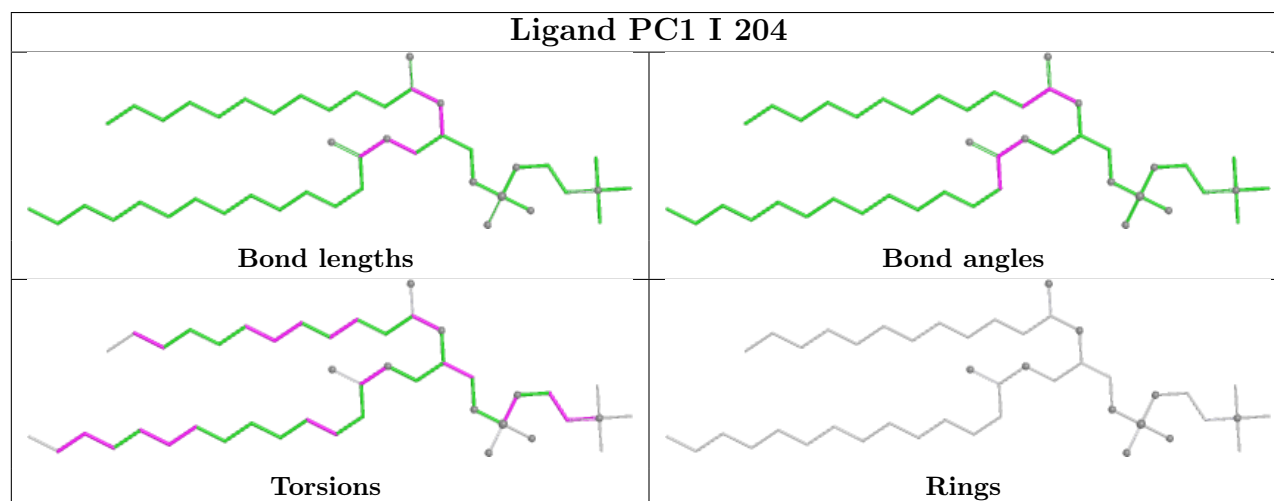
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	I	203	PC1	1	0
46	H	401	PC1	1	0
45	M	603	3PE	1	0
45	Y	205	3PE	1	0
45	m	201	3PE	1	0
45	J	203	3PE	1	0
46	L	706	PC1	1	0
53	M	602	CDL	3	0
45	L	705	3PE	1	0
47	O	403	PLC	1	0
46	A	202	PC1	1	0
53	X	201	CDL	1	0
58	U	101	EHZ	1	0
59	i	201	CHD	4	0
49	D	501	U10	22	0
46	g	202	PC1	1	0
55	O	401	DGT	3	0
48	B	201	SF4	1	0

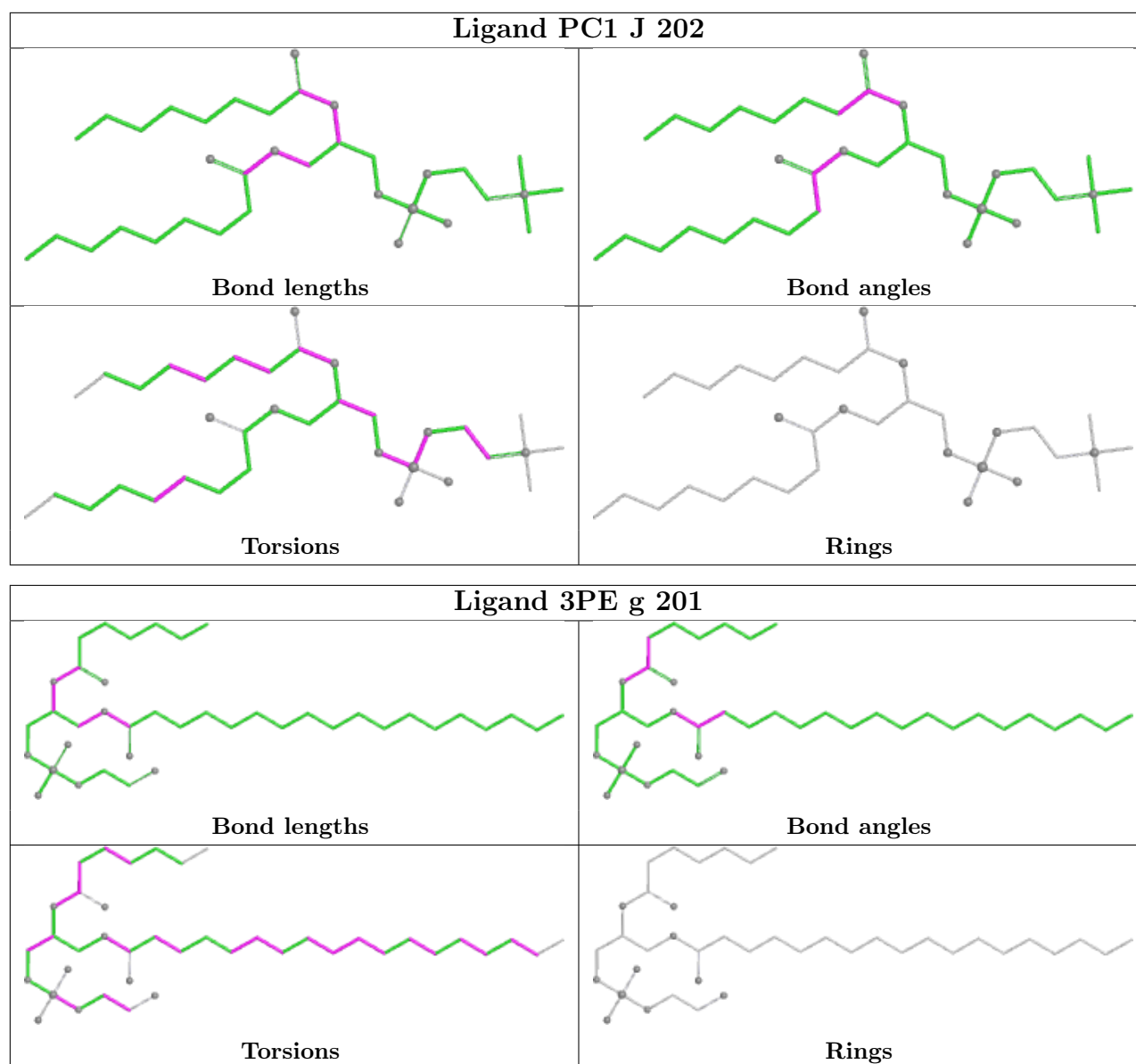
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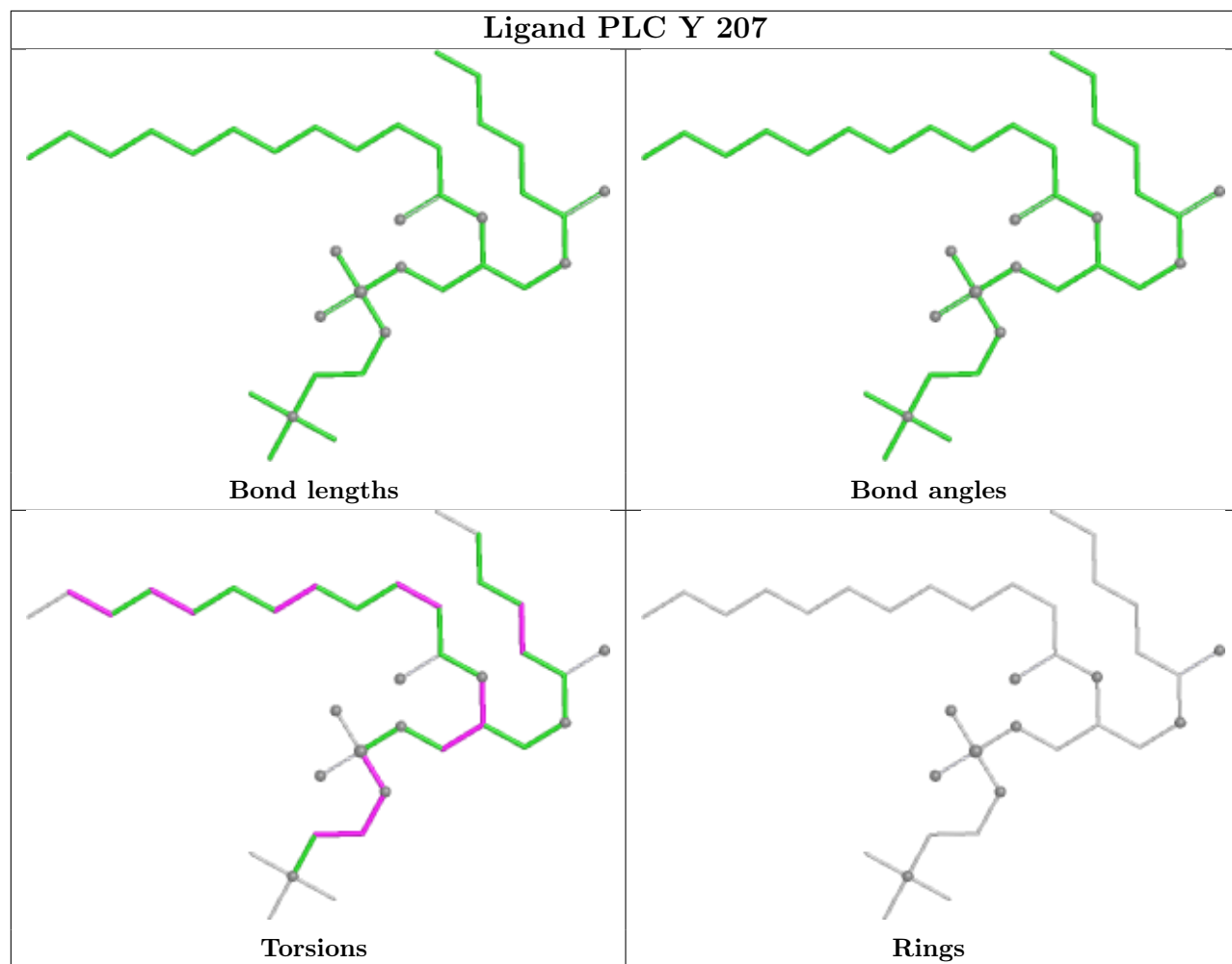
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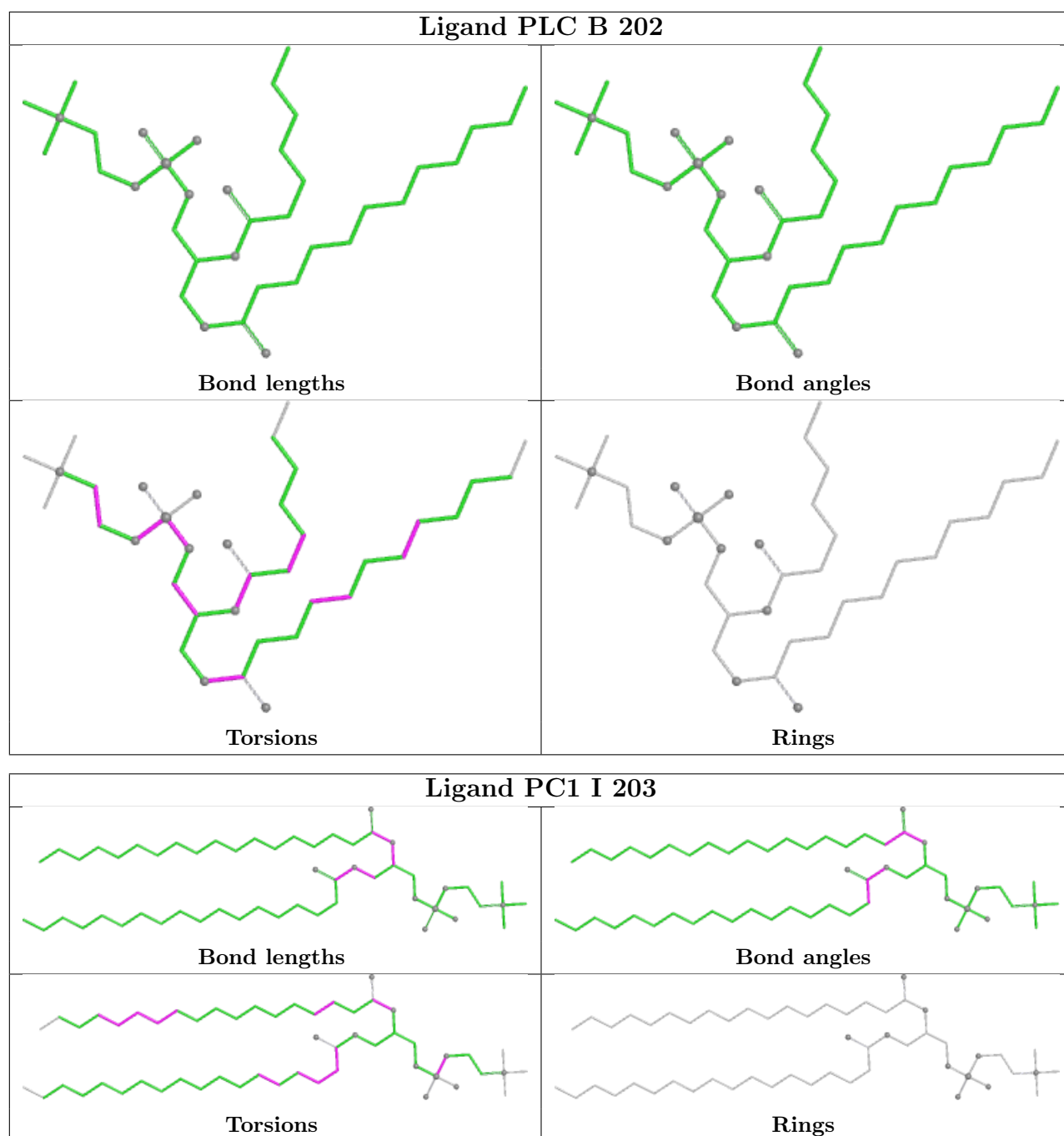
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	A	206	PLC	1	0
53	P	502	CDL	1	0
47	P	505	PLC	1	0
45	a	101	3PE	1	0
58	T	101	EHZ	1	0
53	i	202	CDL	1	0
53	d	201	CDL	2	0
45	J	206	3PE	1	0
45	Y	203	3PE	1	0
46	B	203	PC1	1	0
51	F	501	FMN	1	0

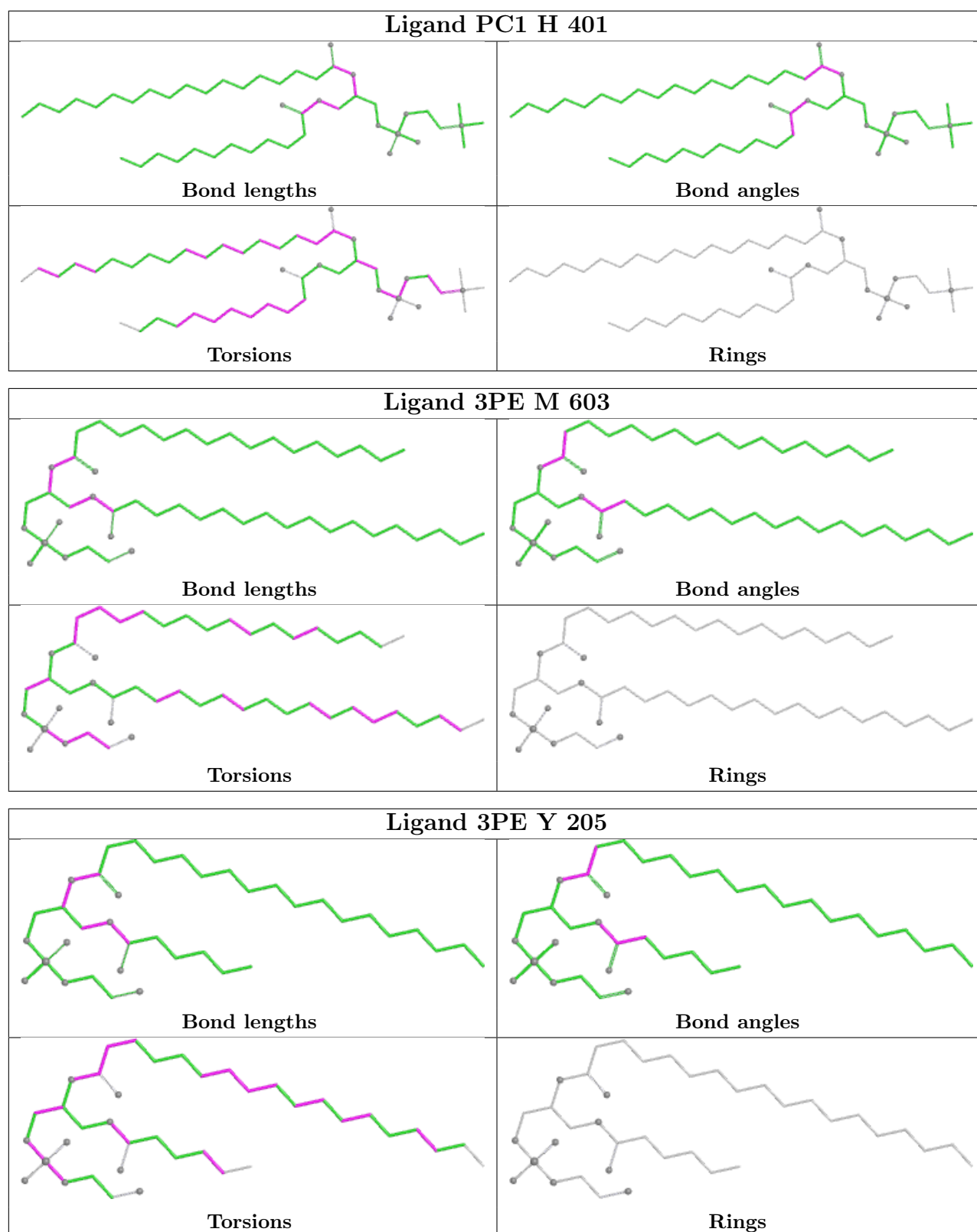
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

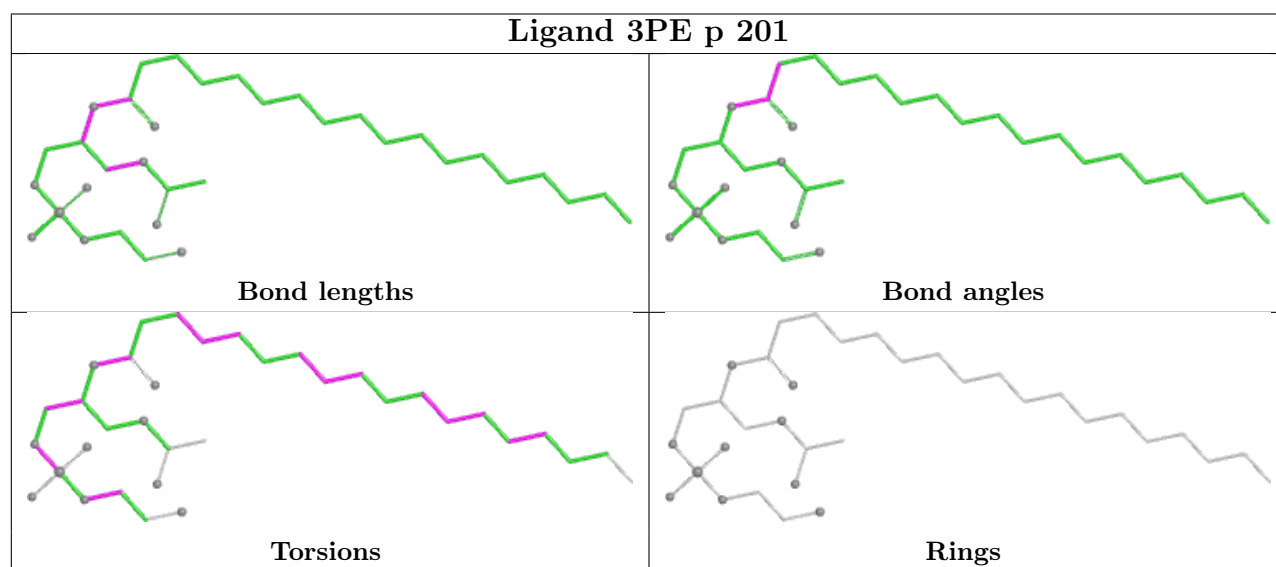
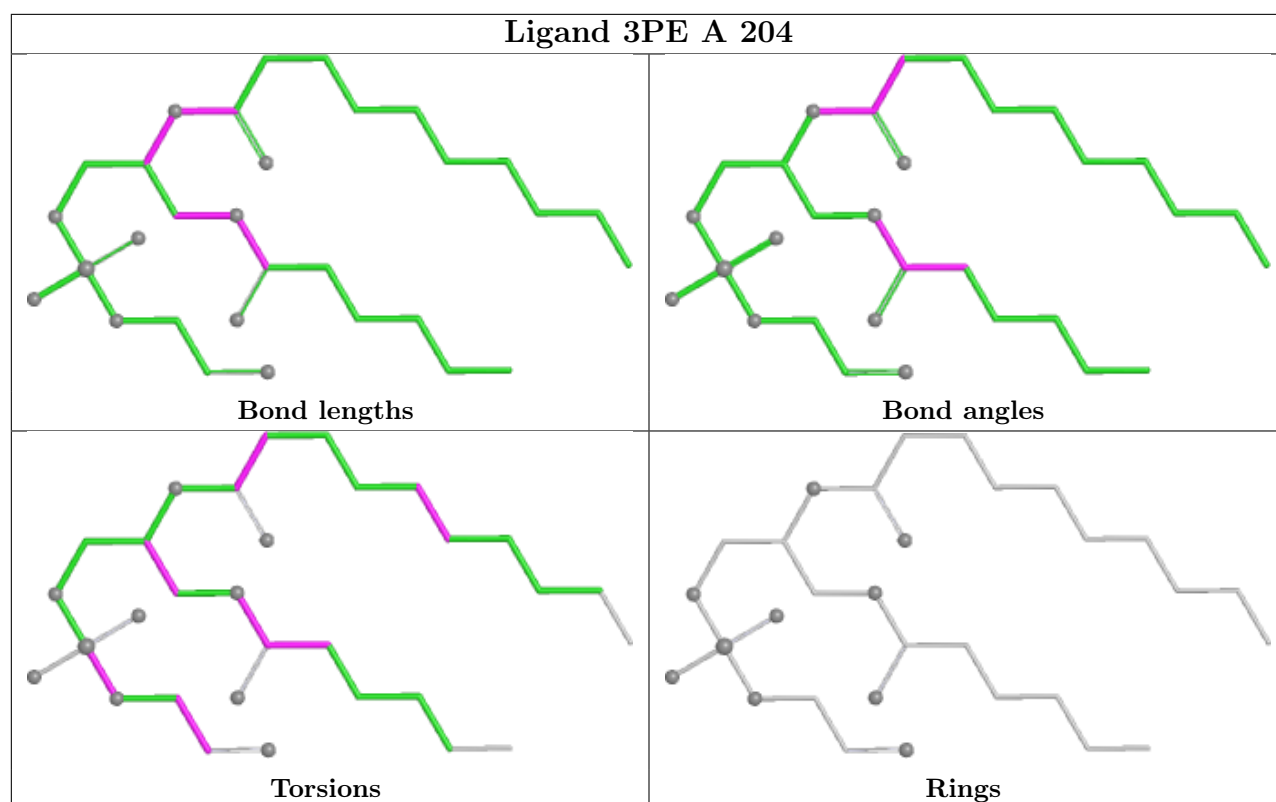


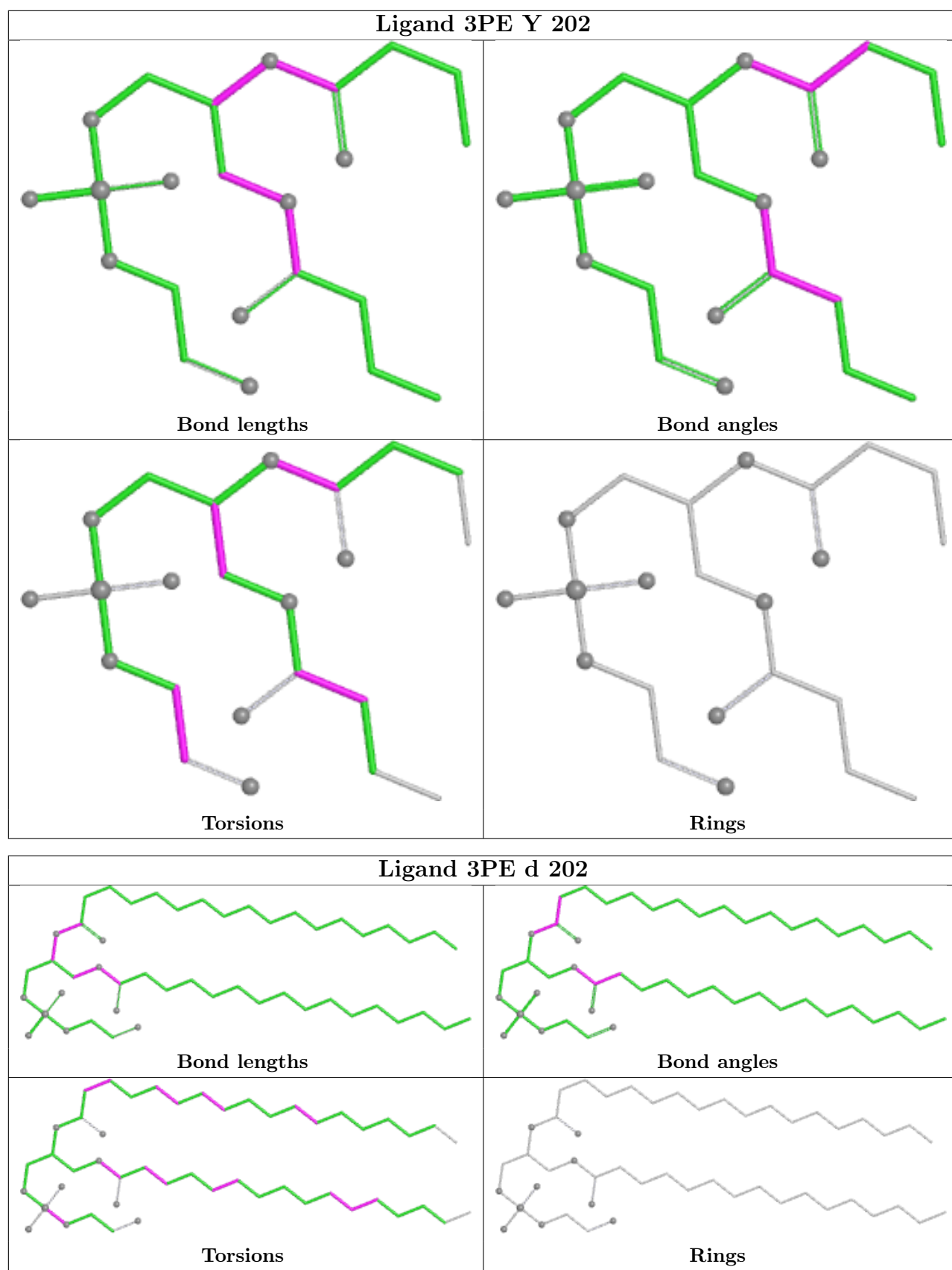


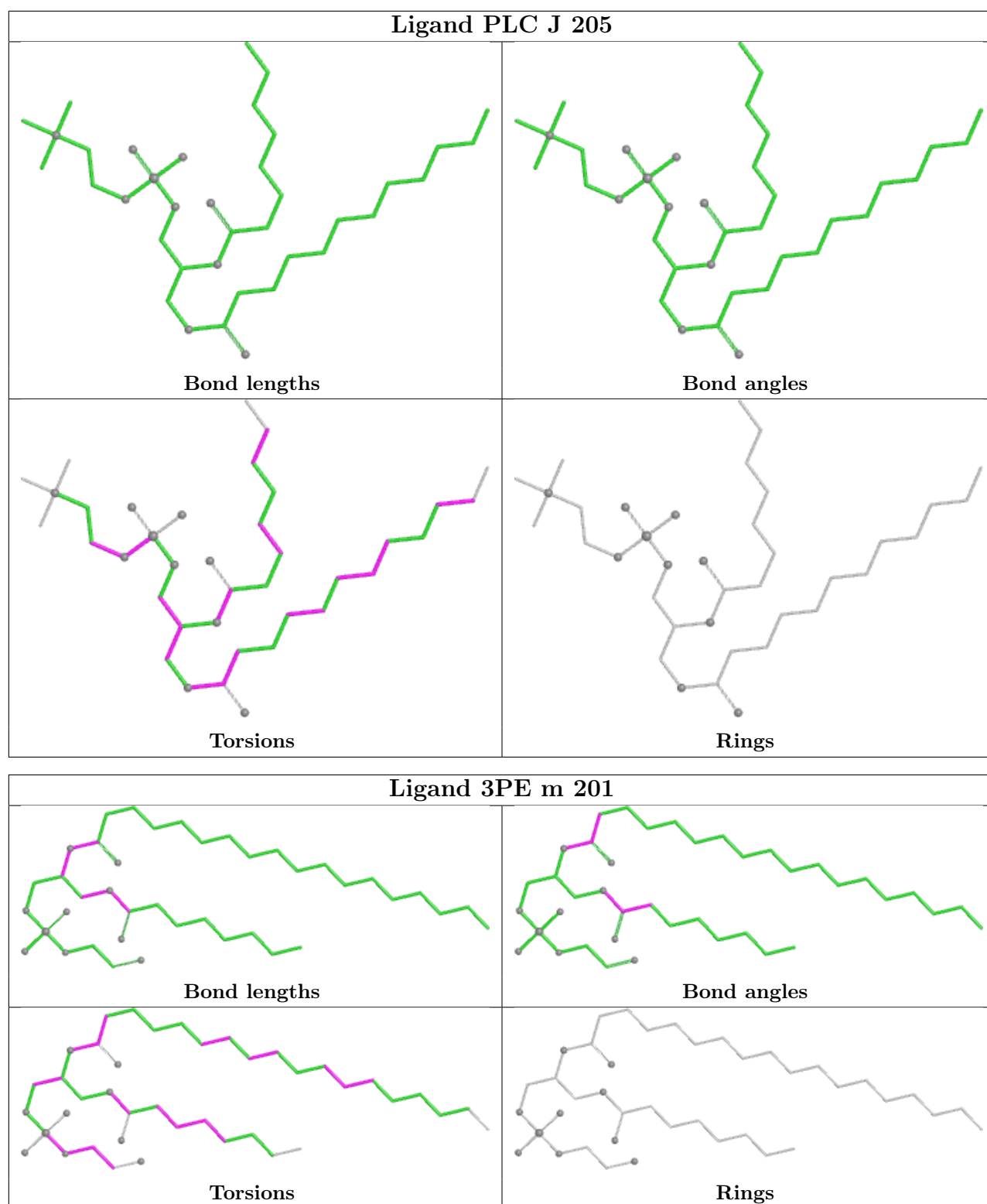


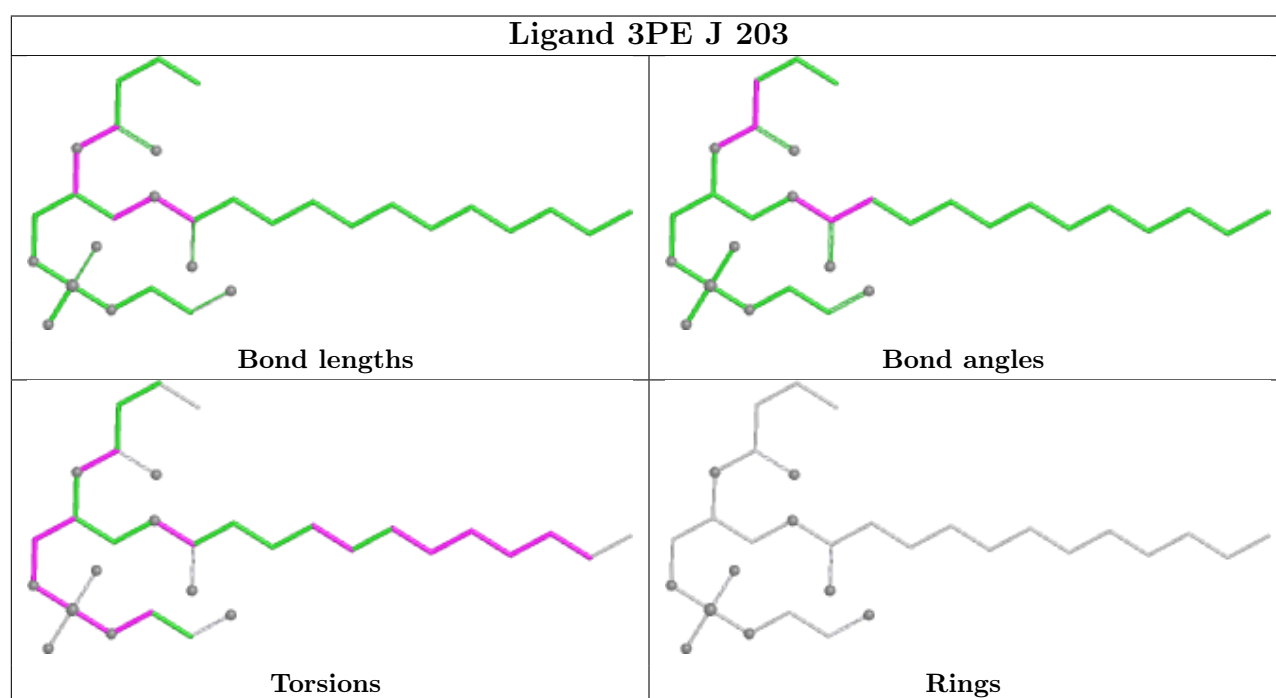
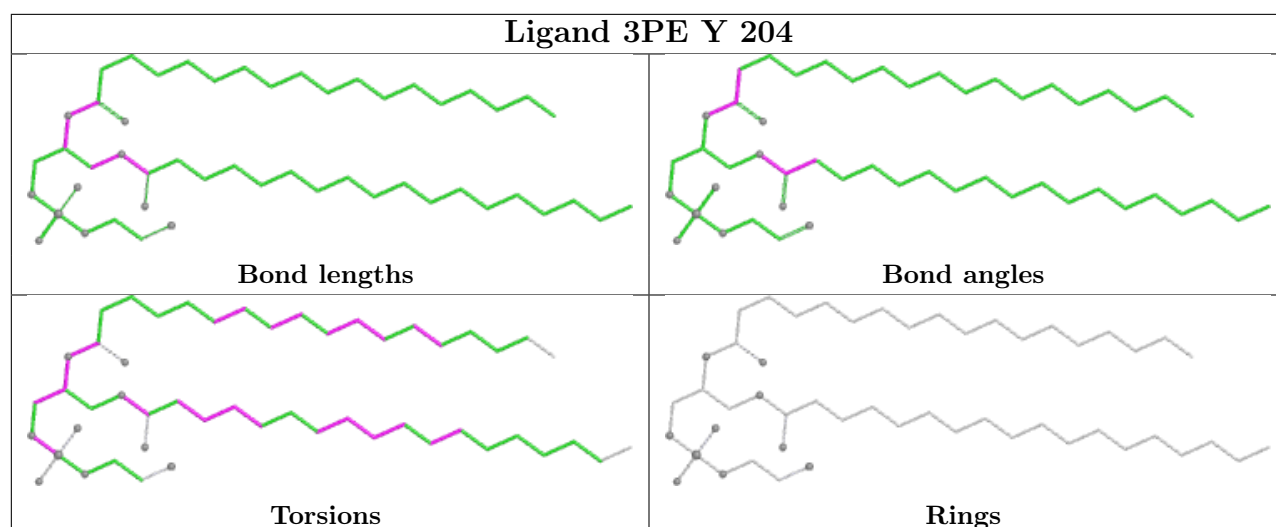


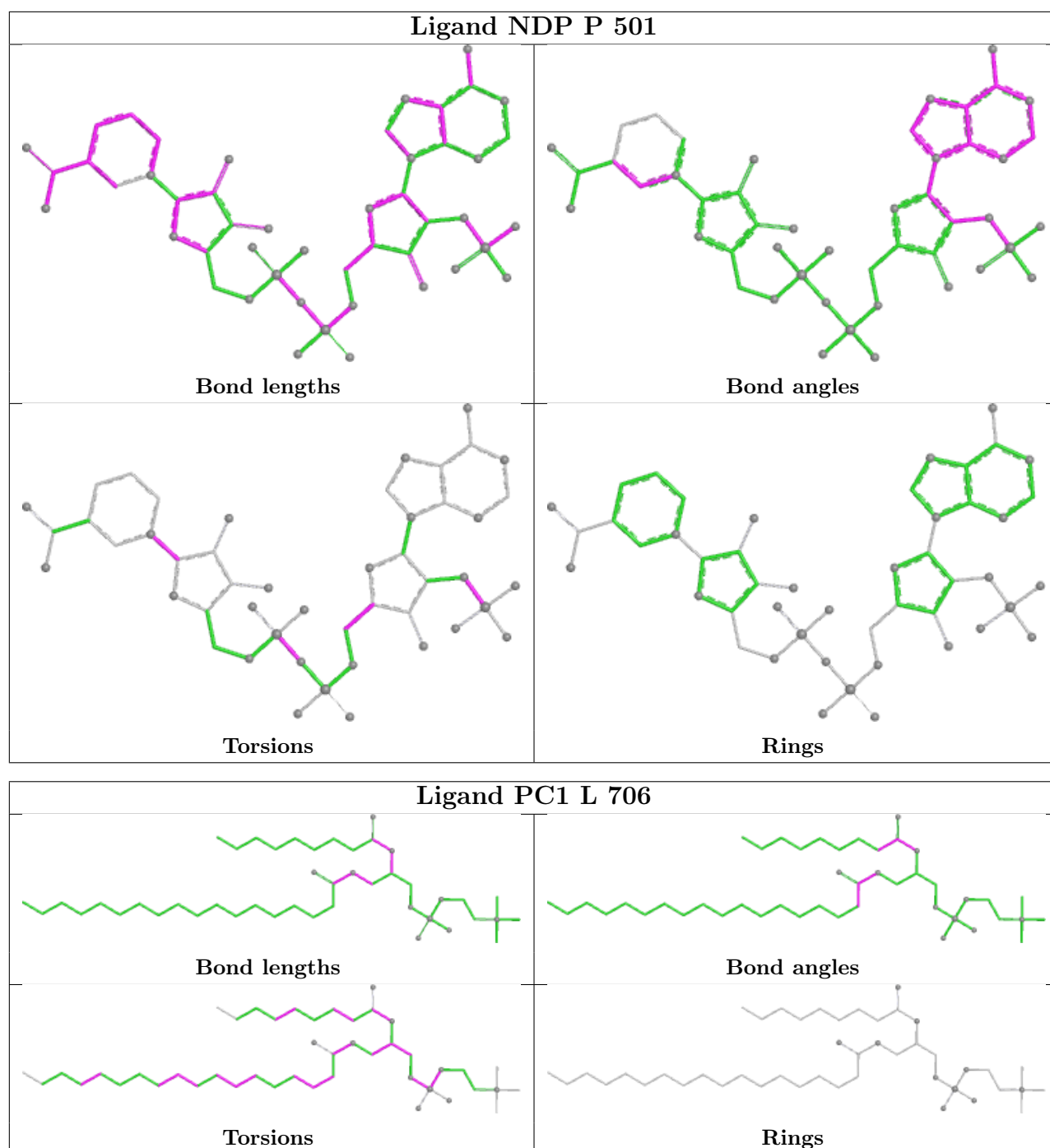


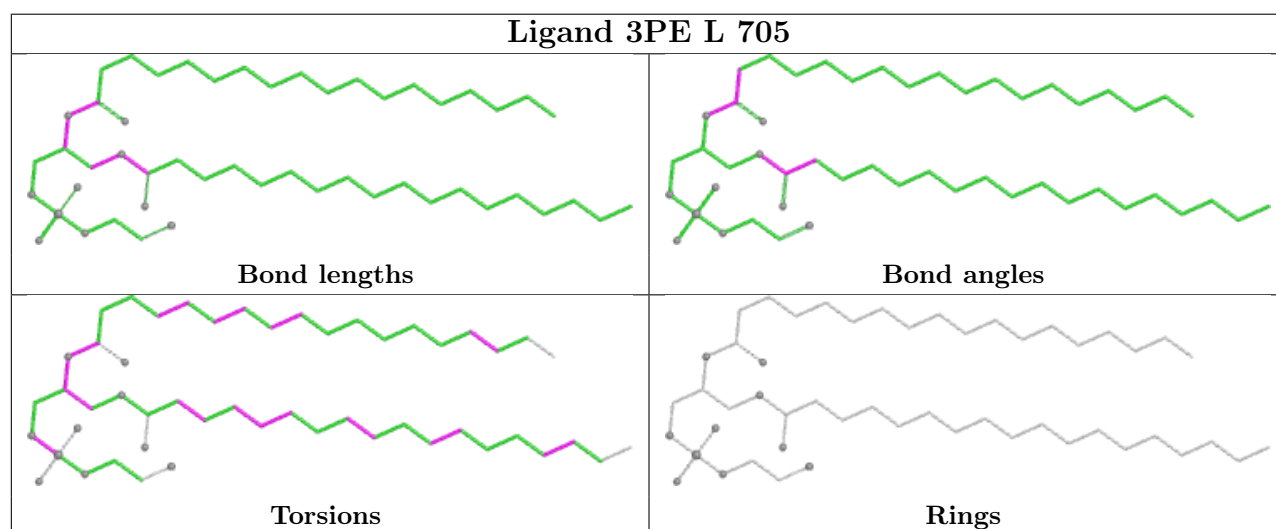
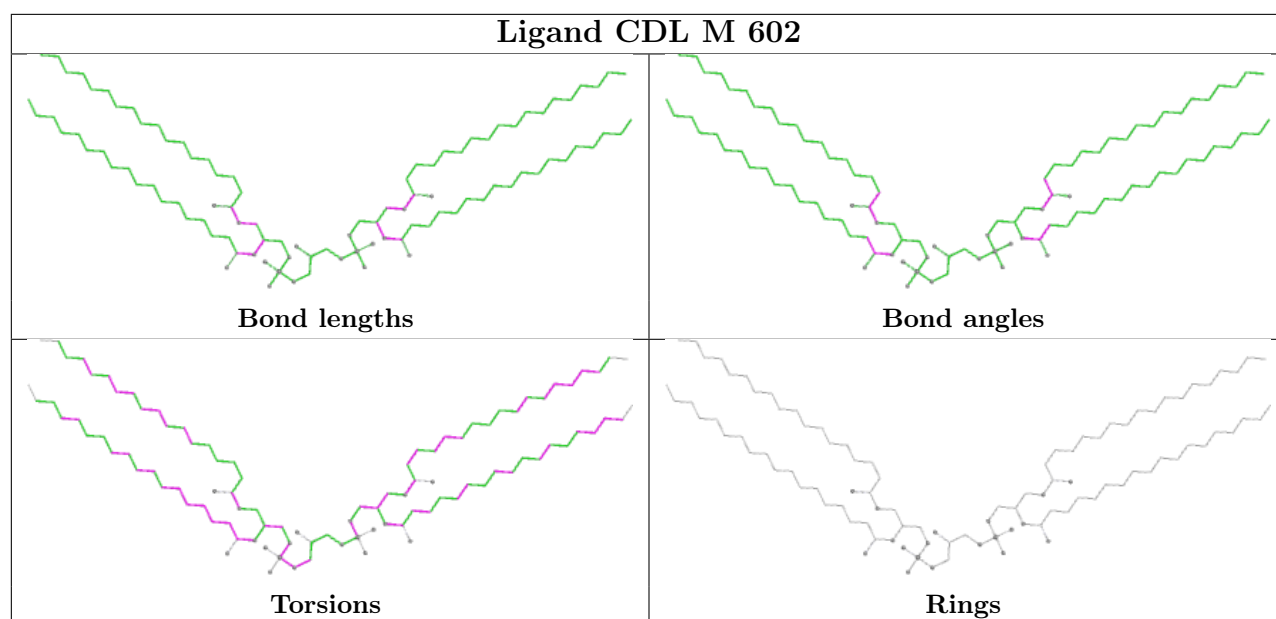


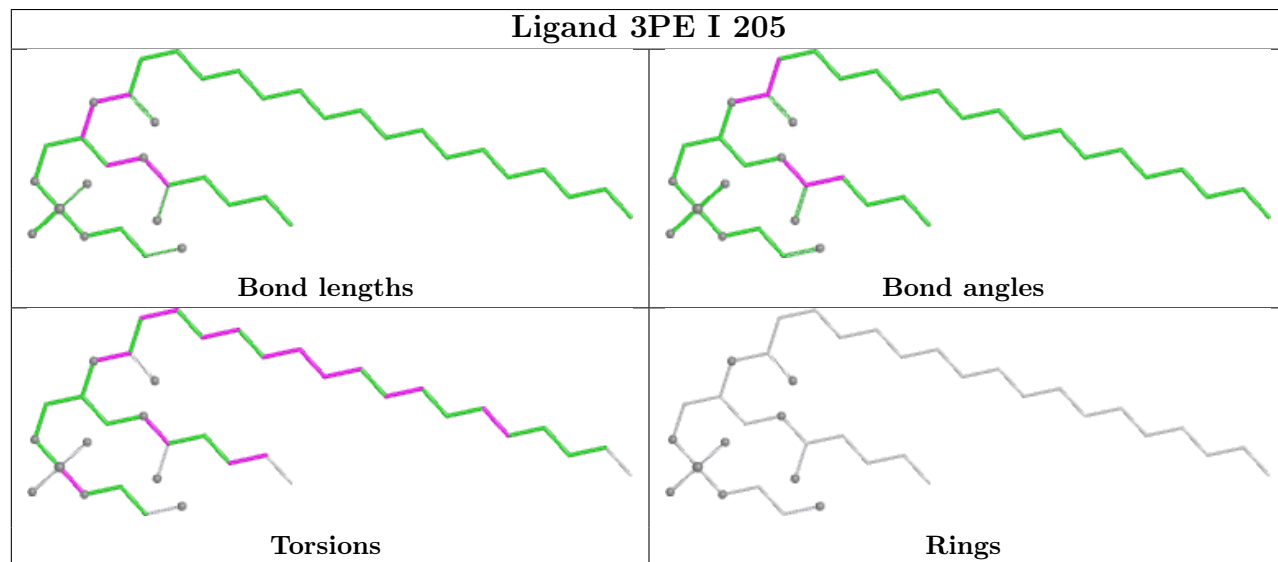
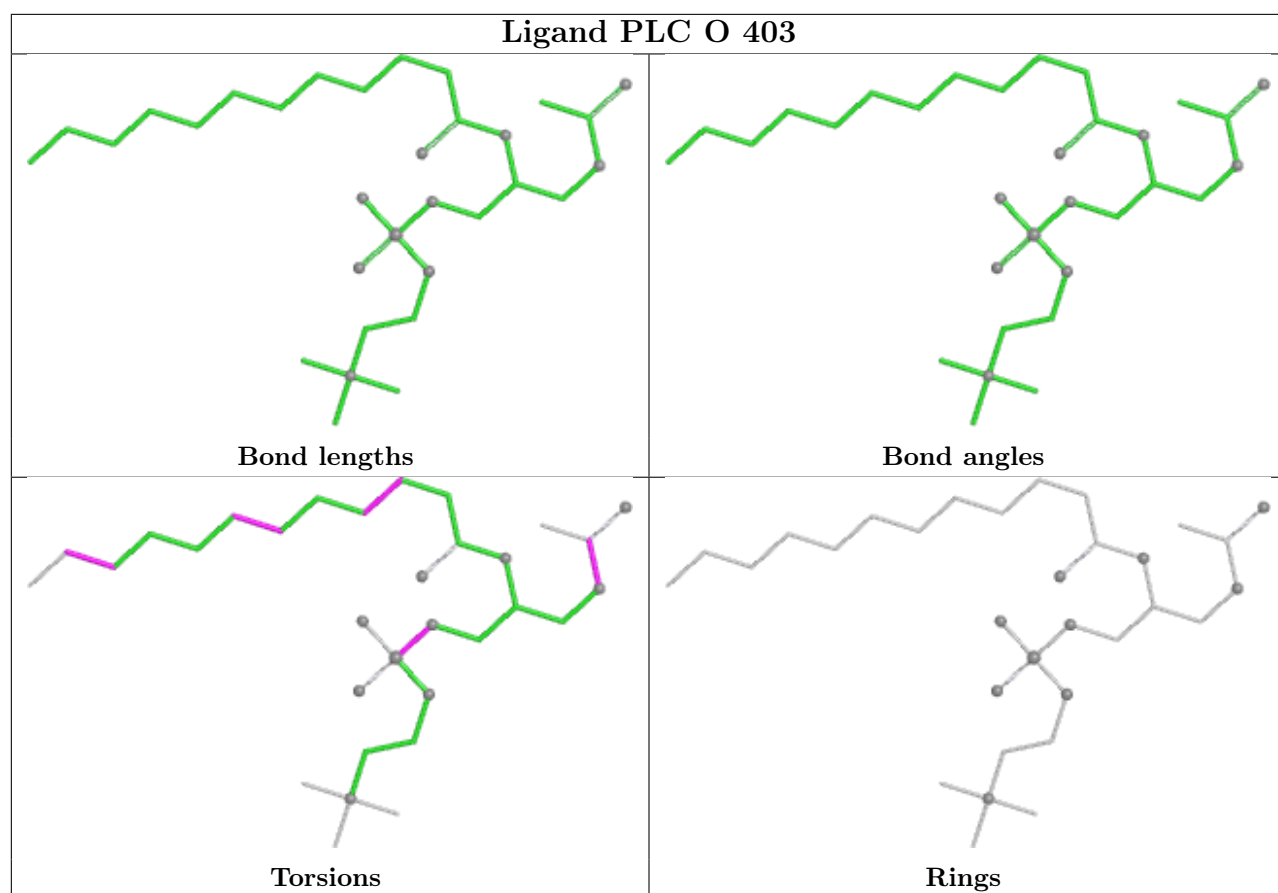


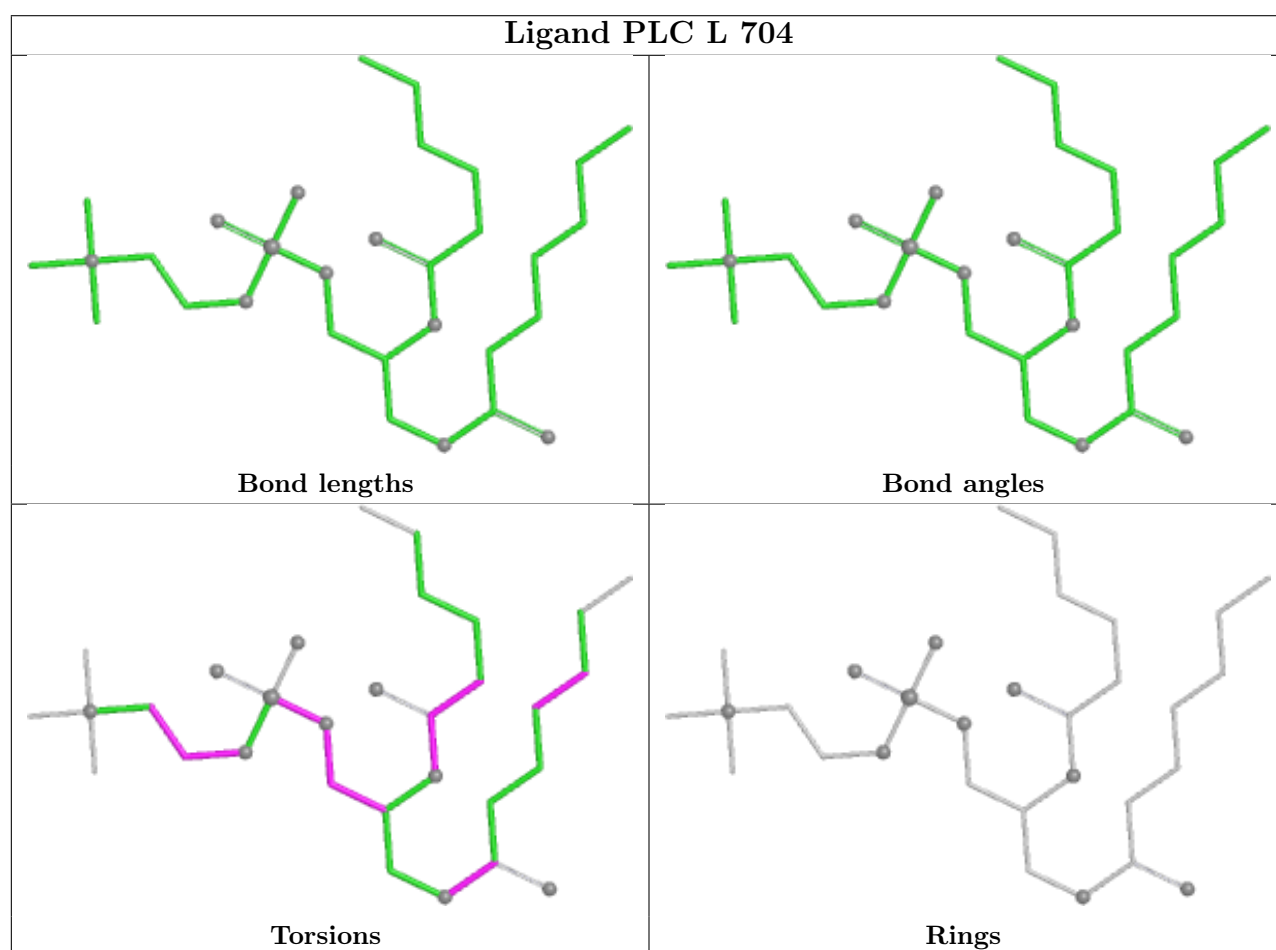
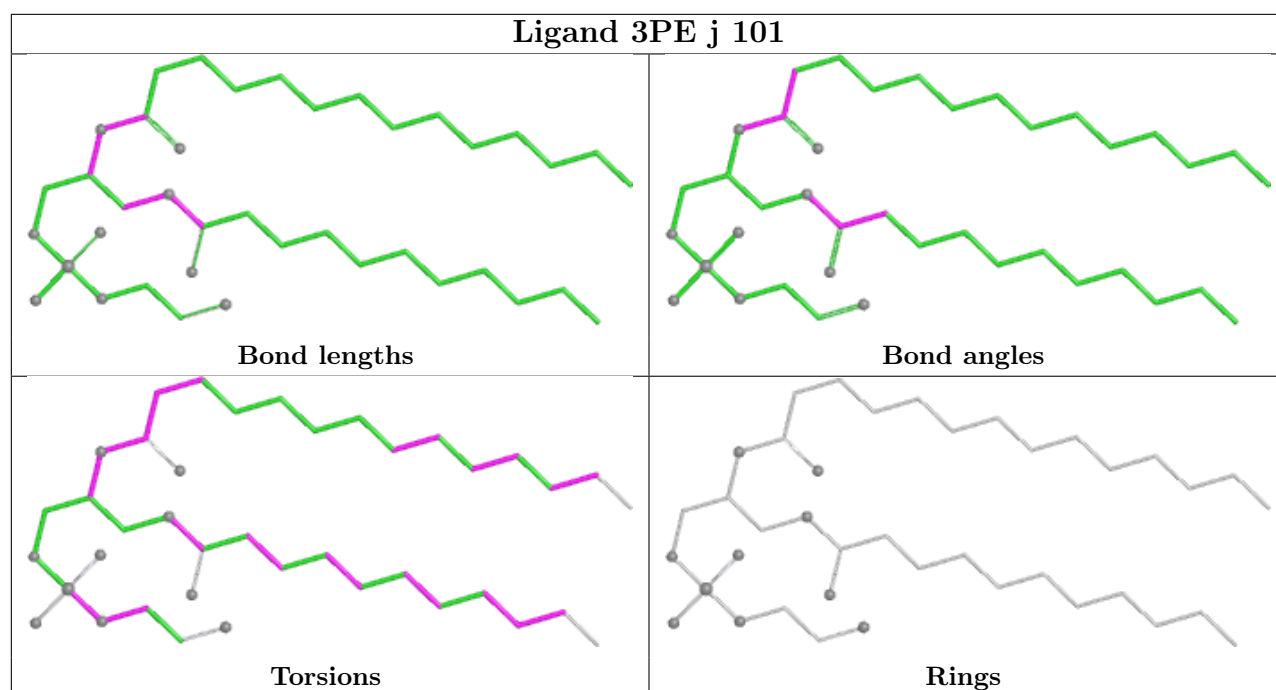


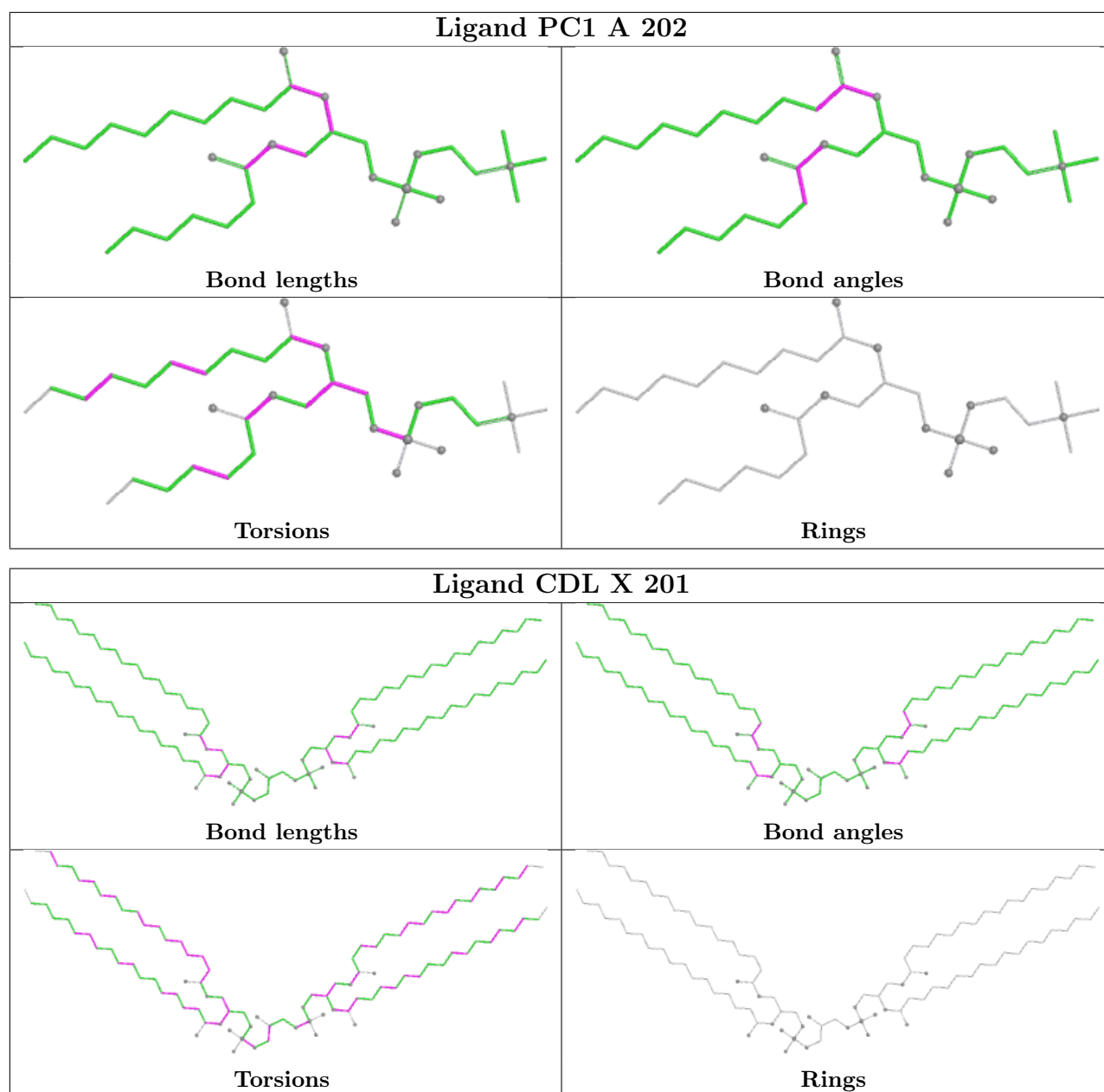


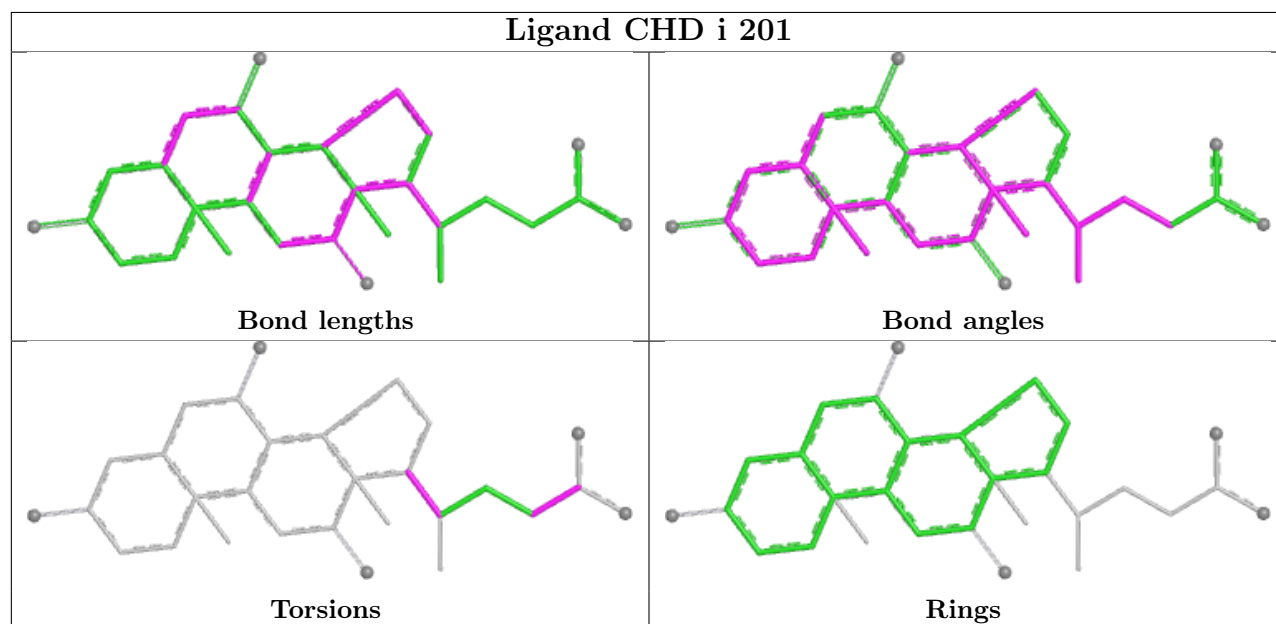
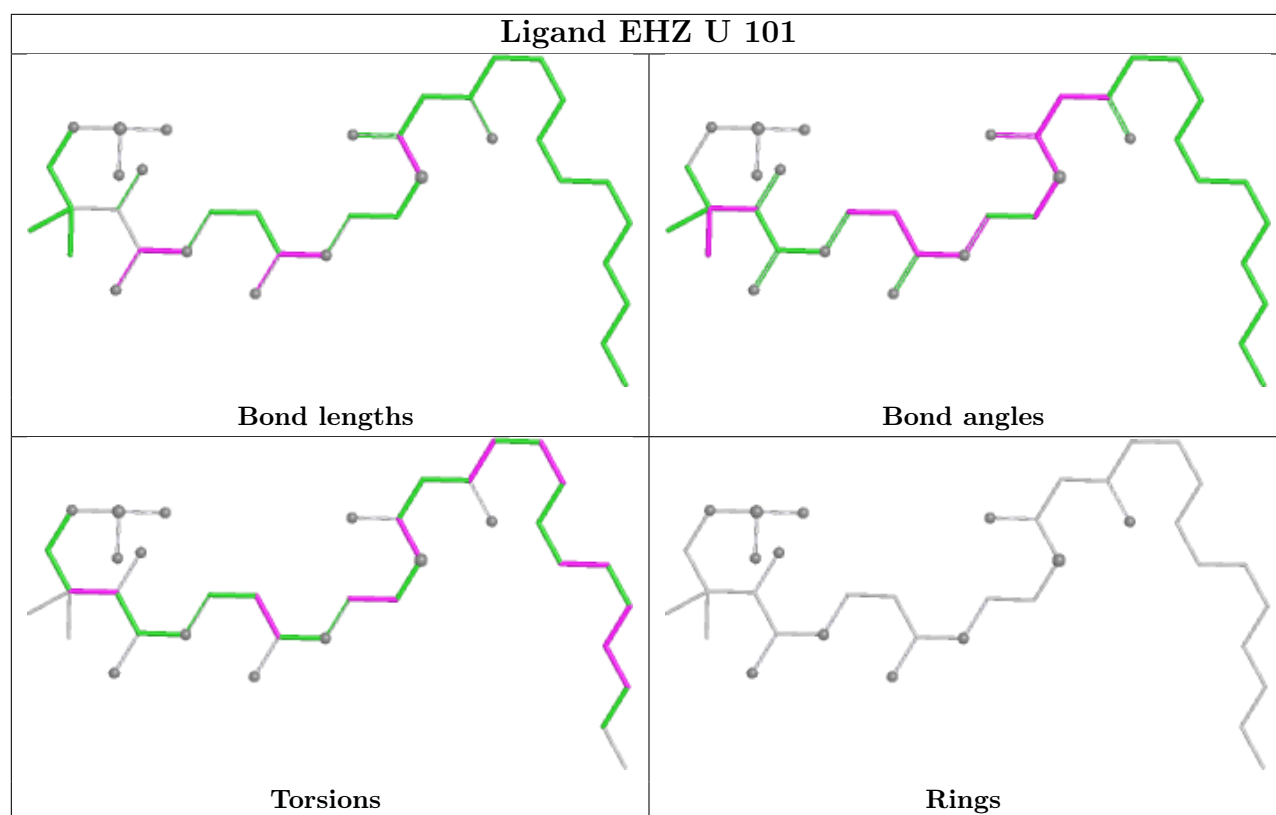


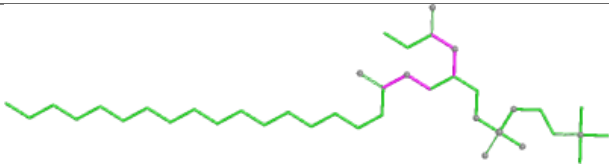
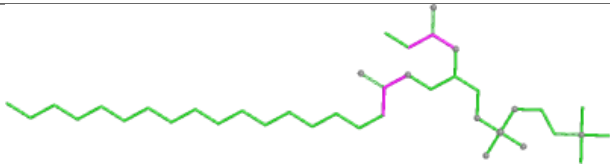
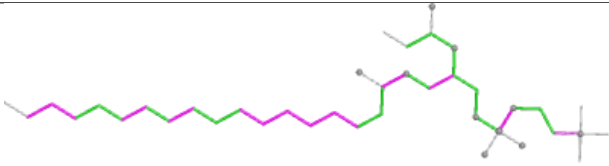
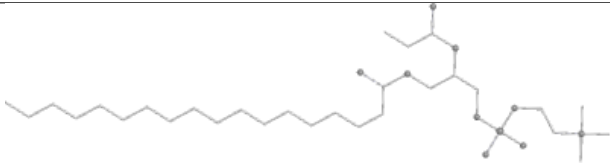


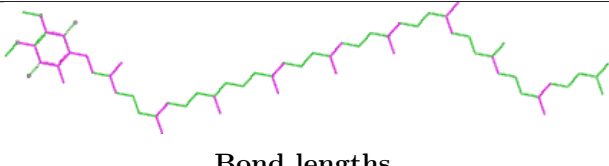
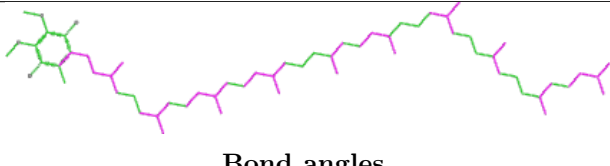
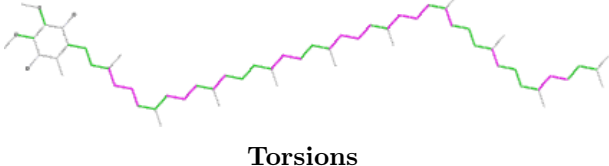


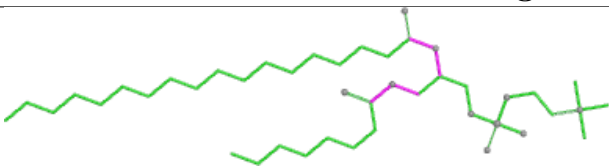
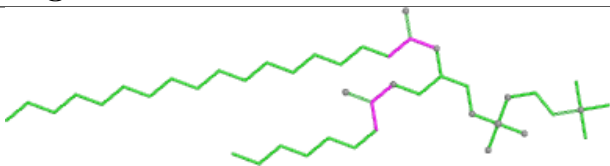
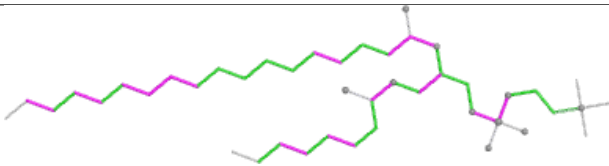
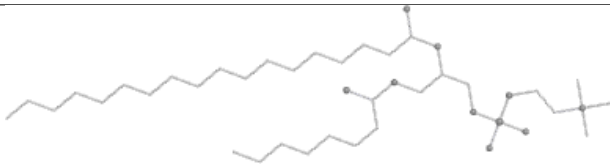


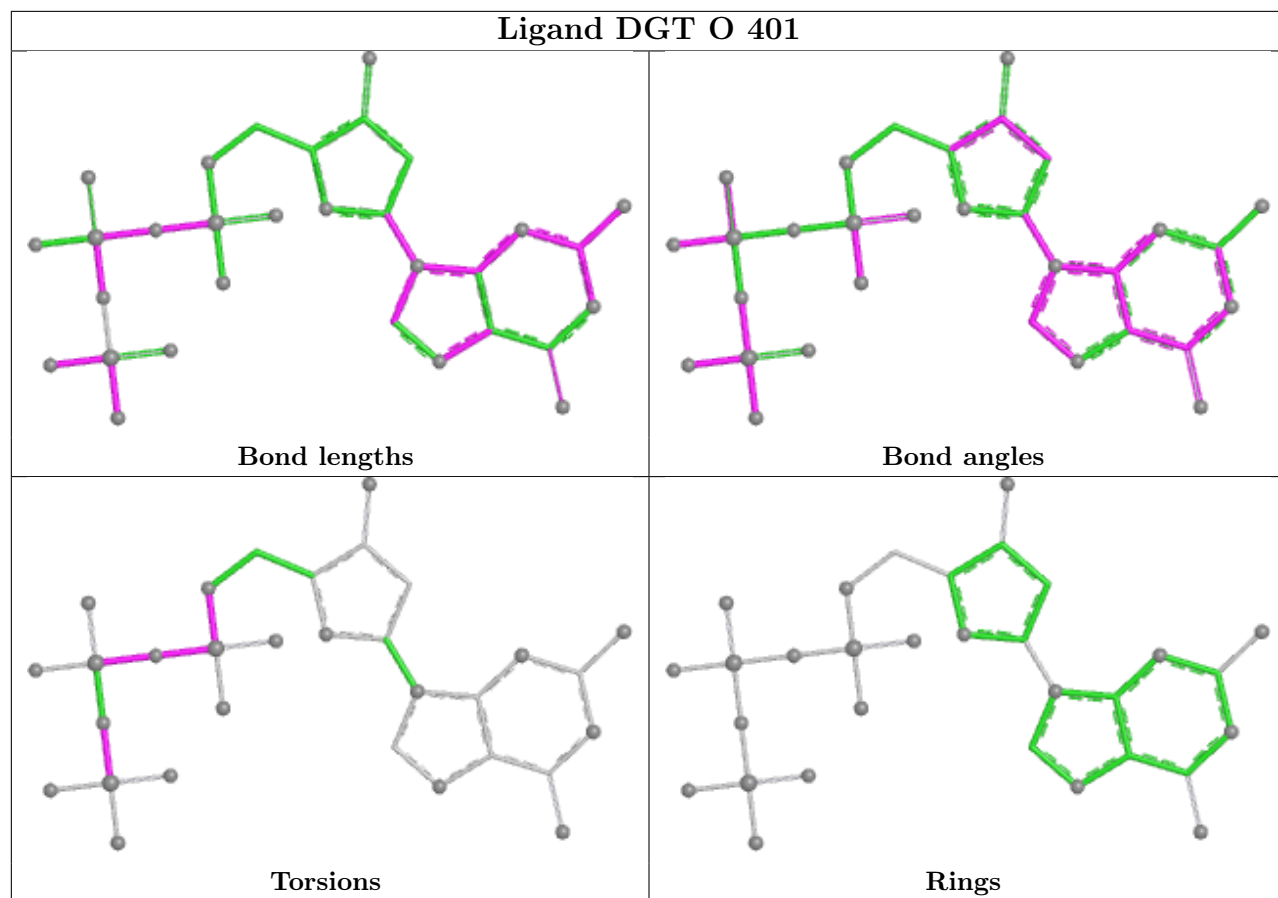




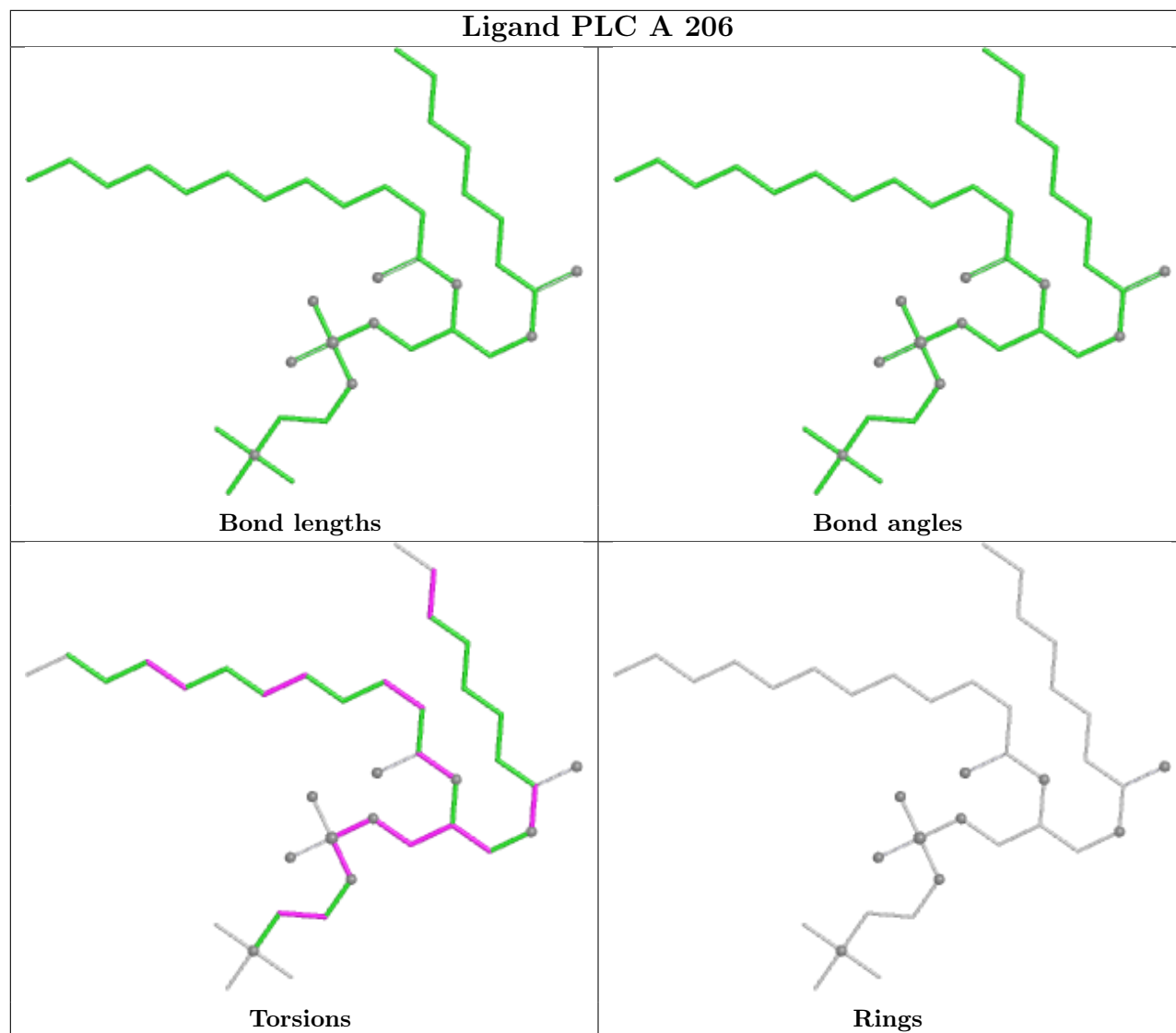
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 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U10 D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

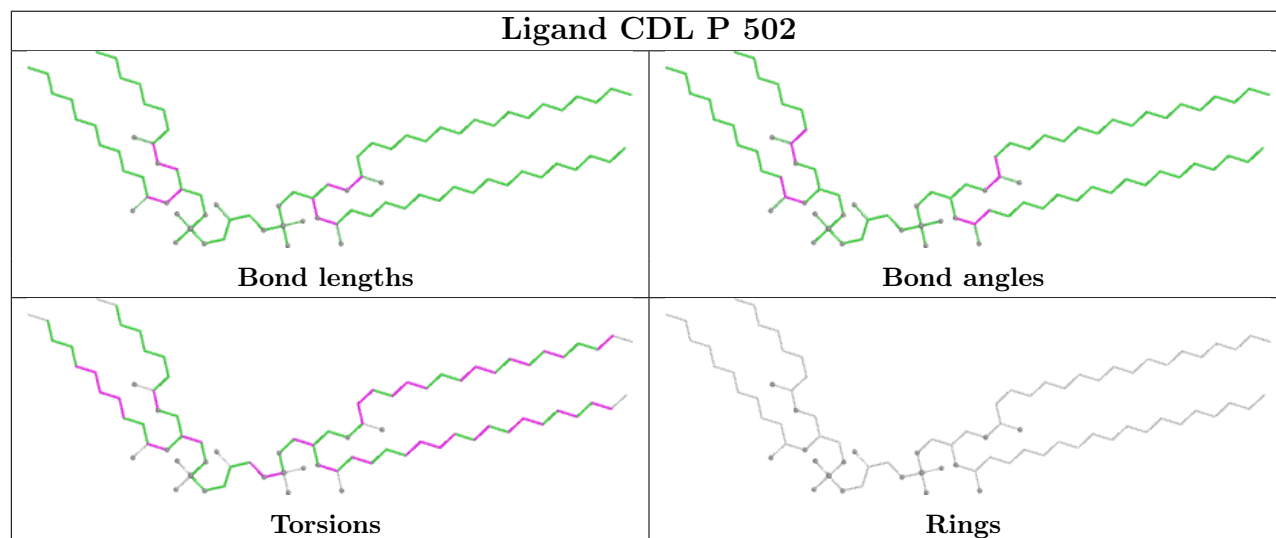
Ligand PC1 g 202	
 Bond lengths	 Bond angles
 Torsions	 Rings



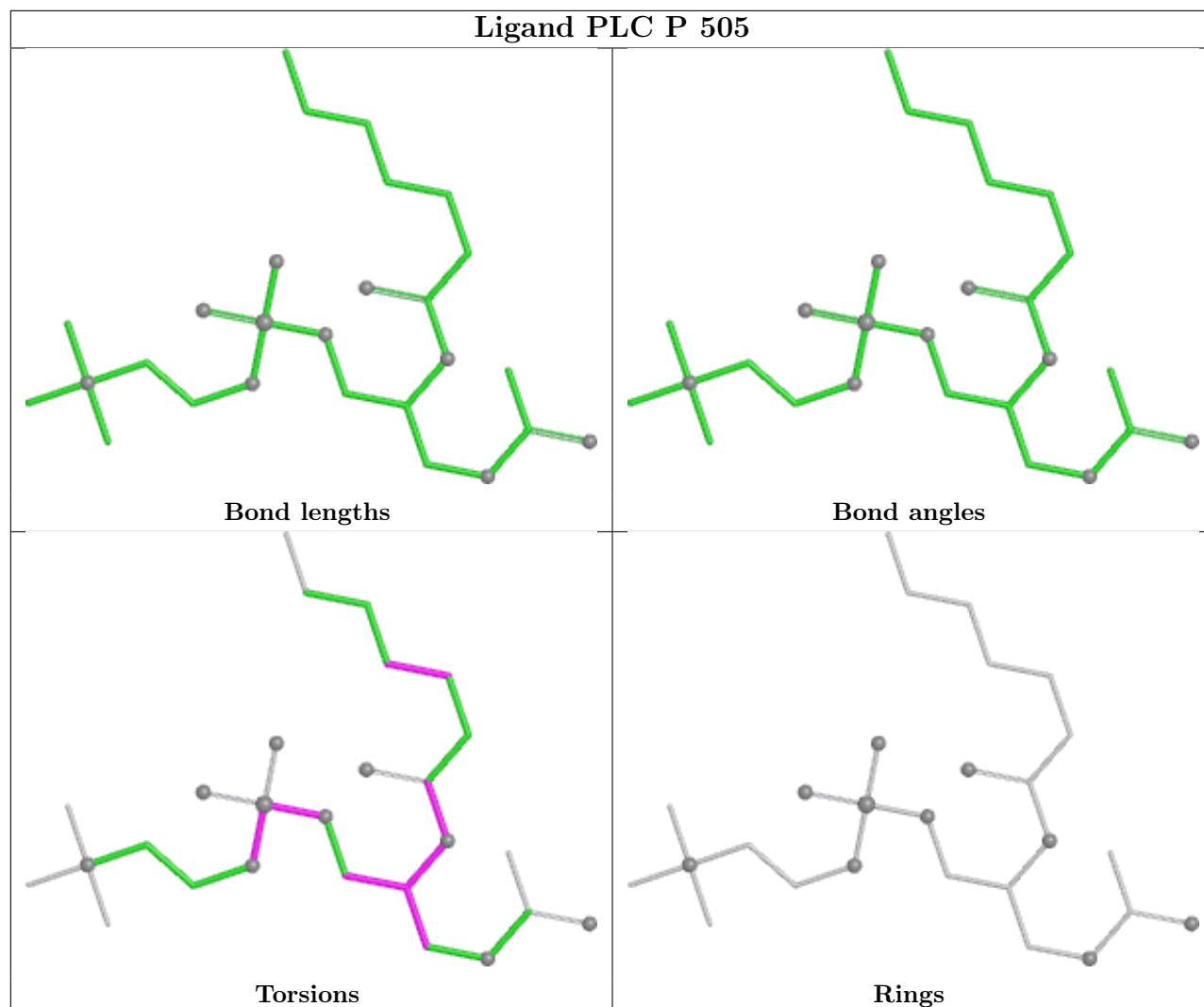
Ligand PLC A 206



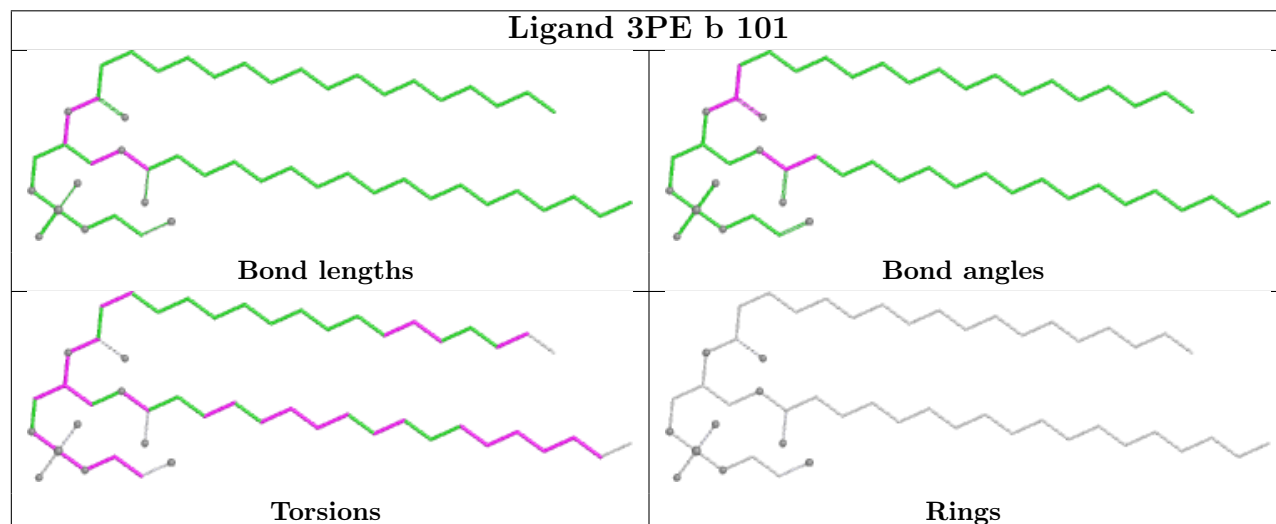
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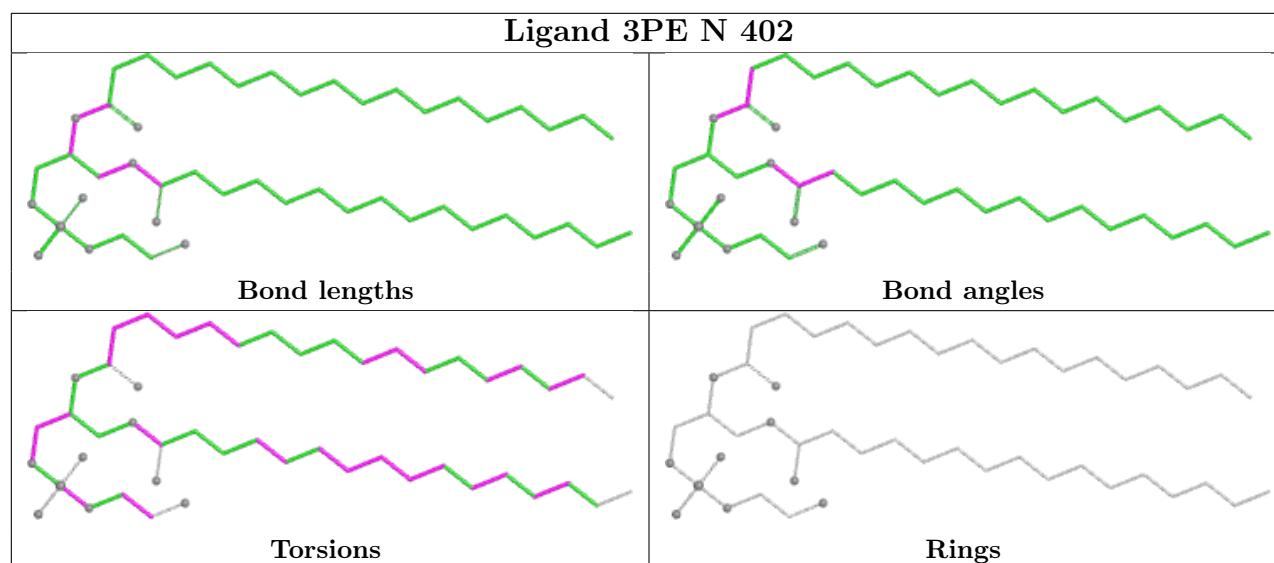
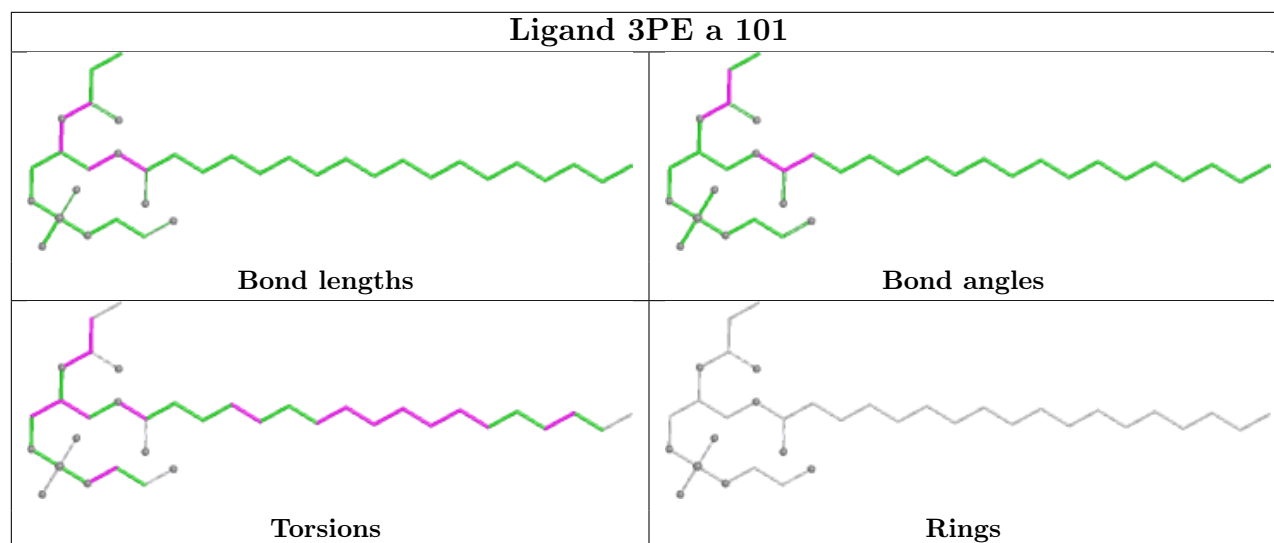
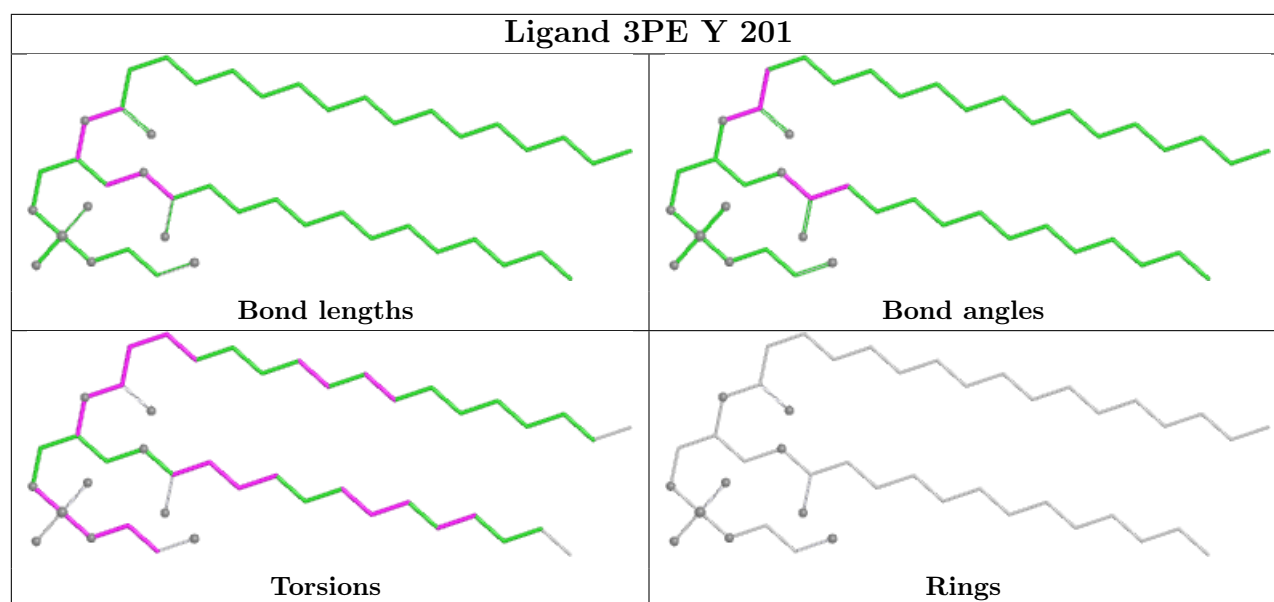


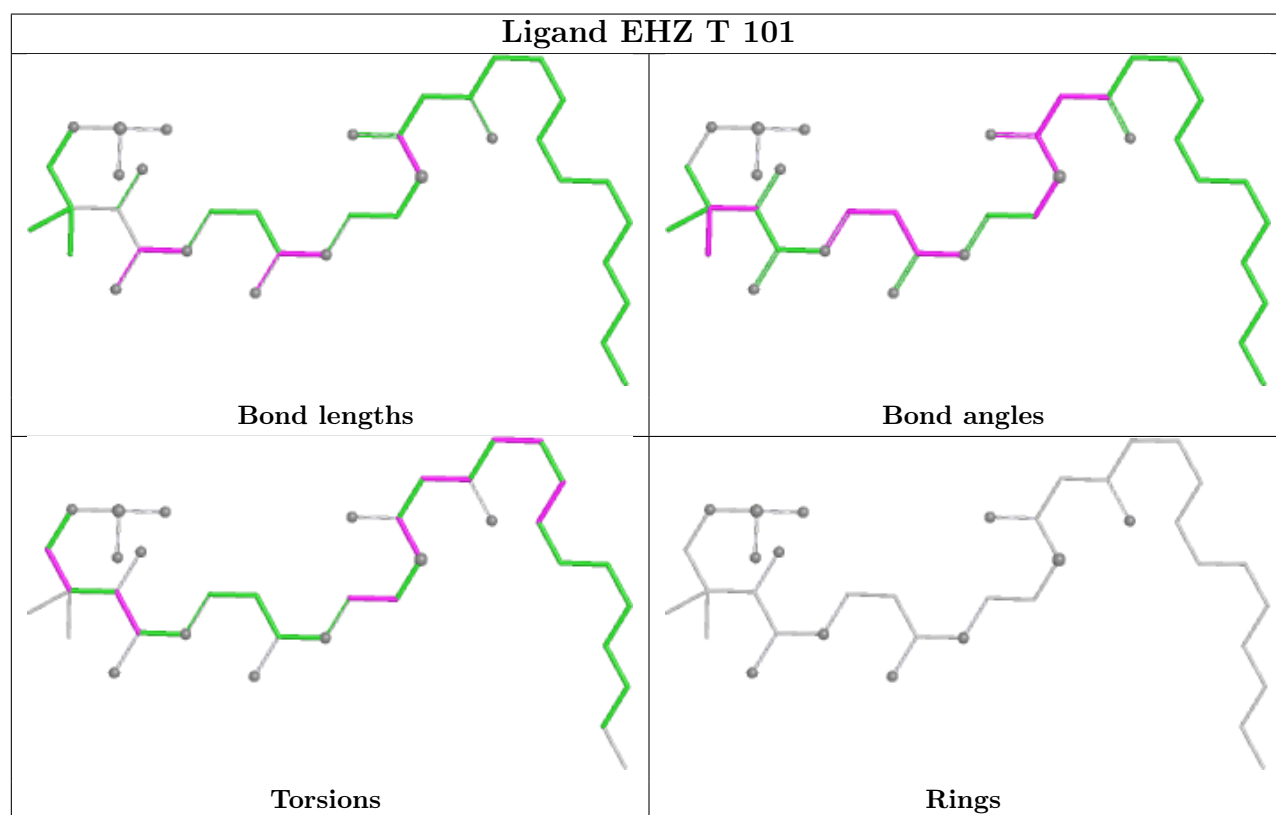
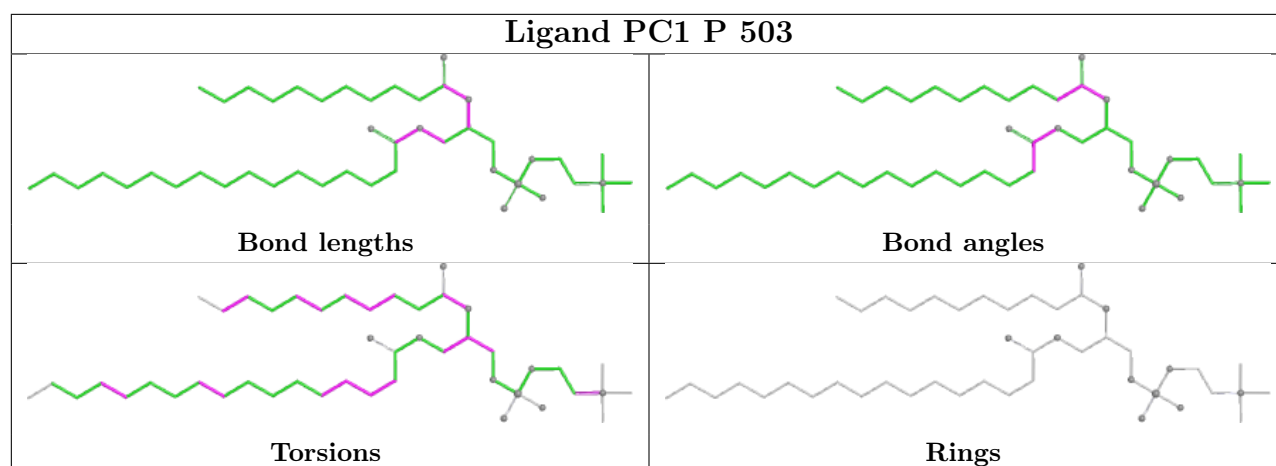
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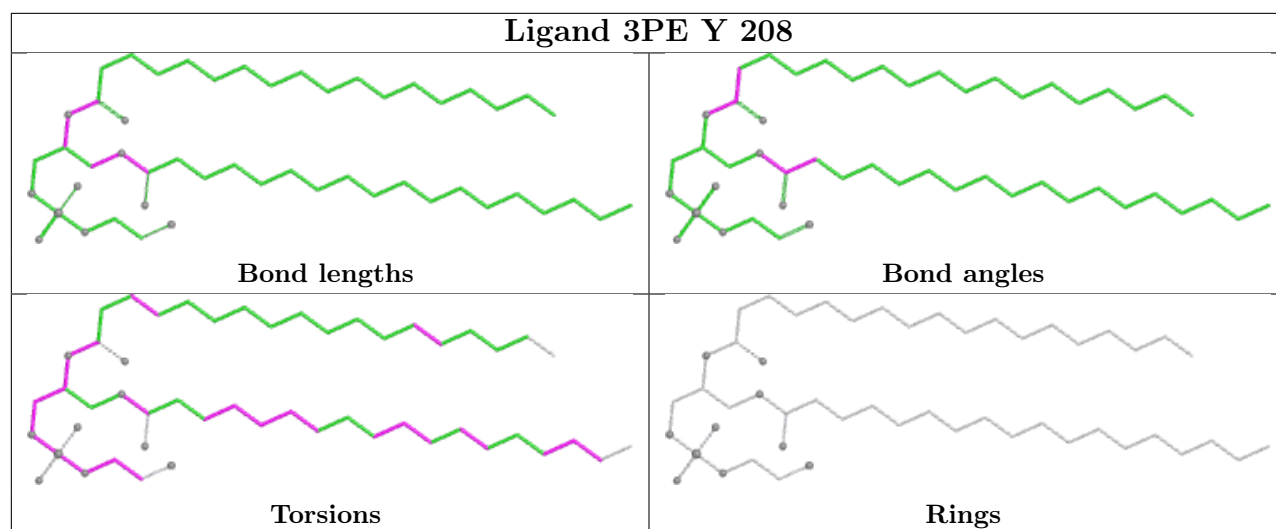
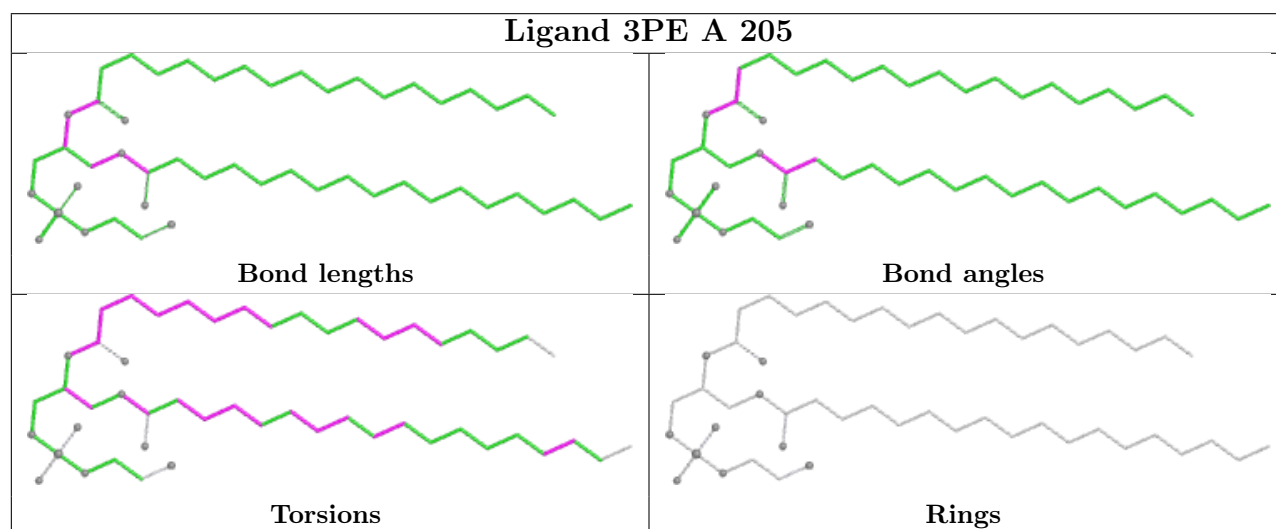
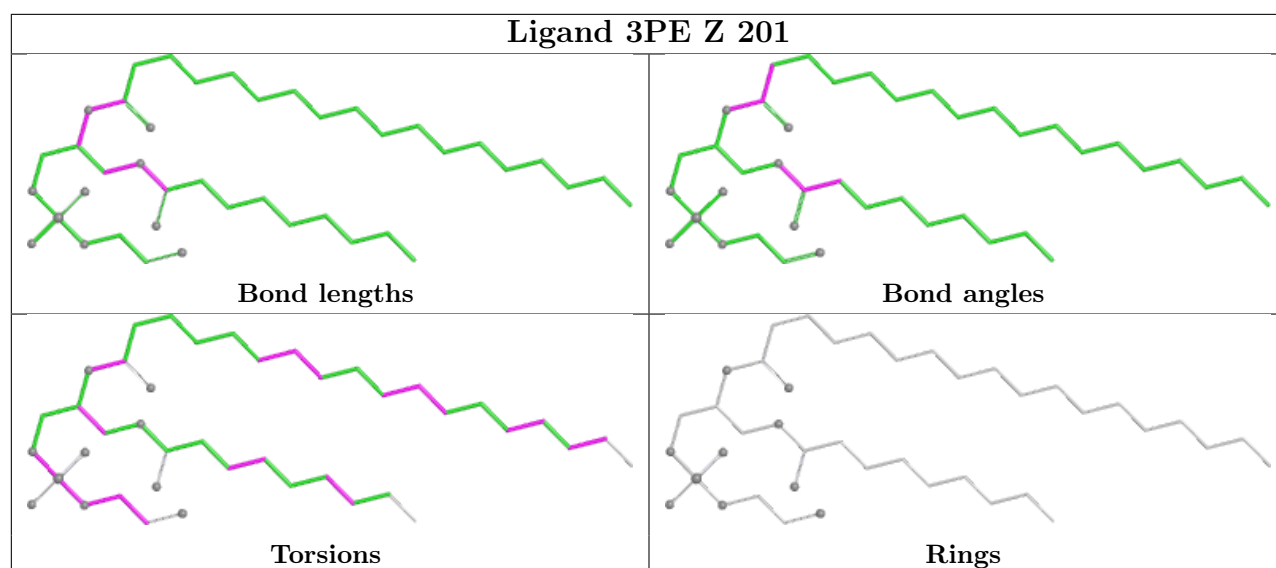


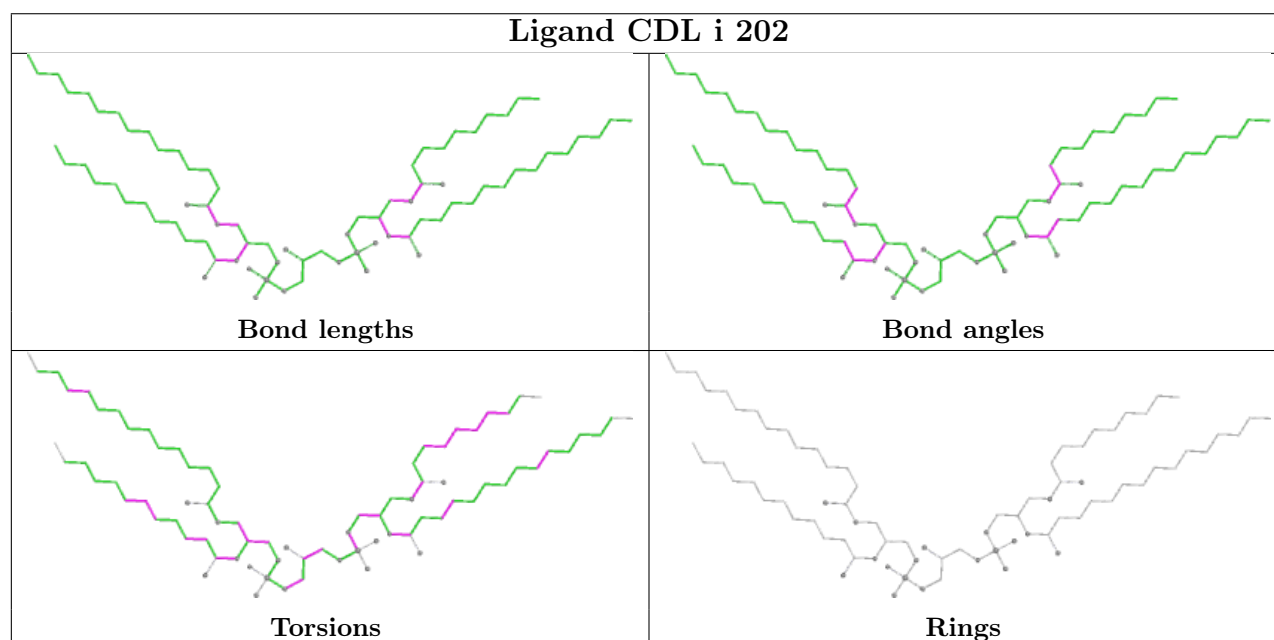
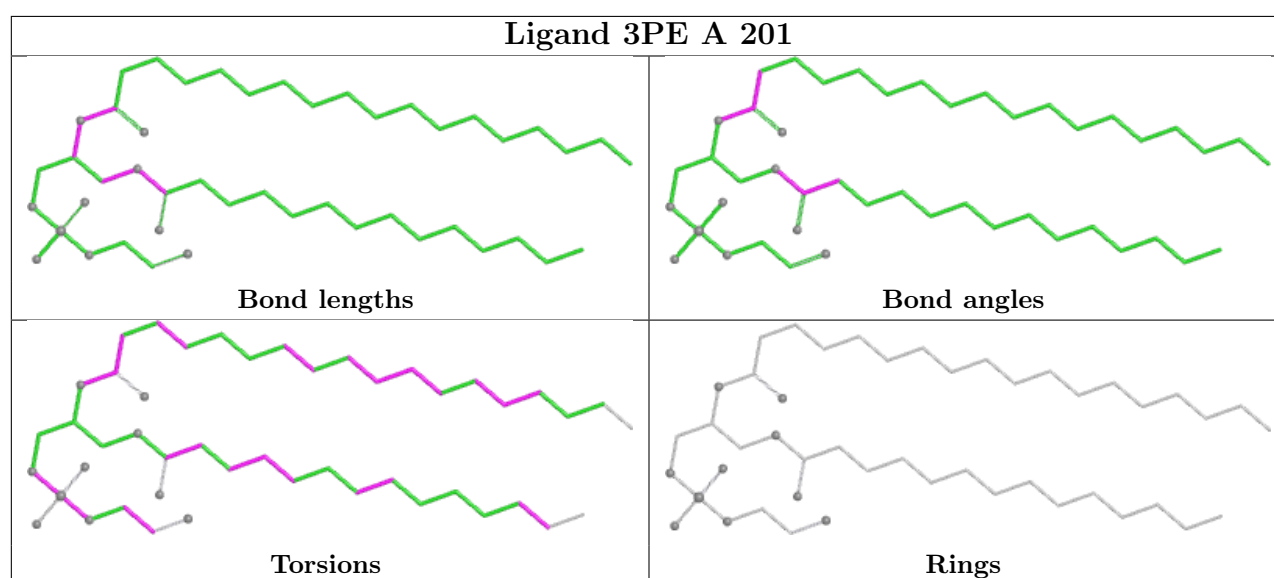
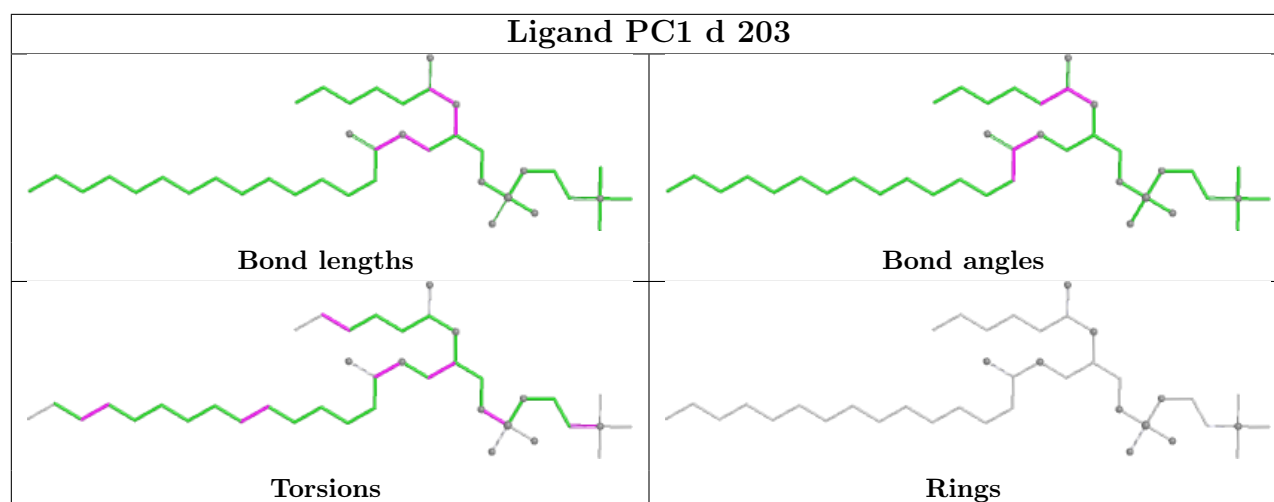
Ligand 3PE b 101

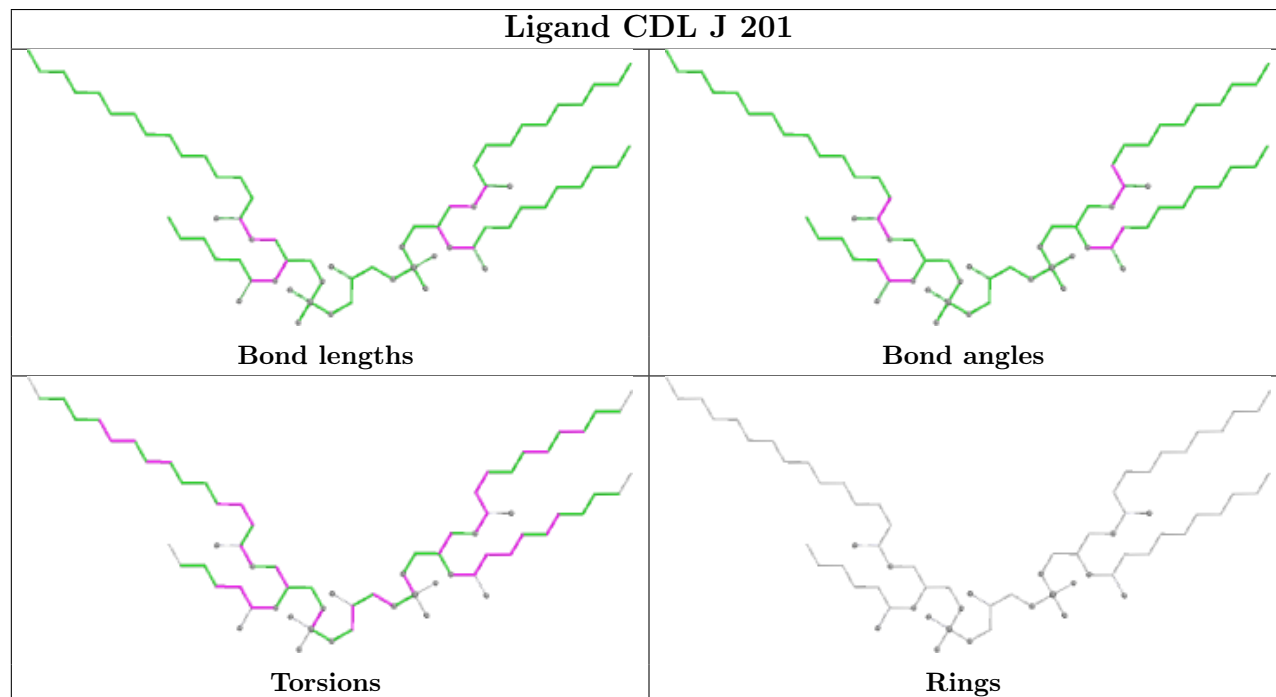
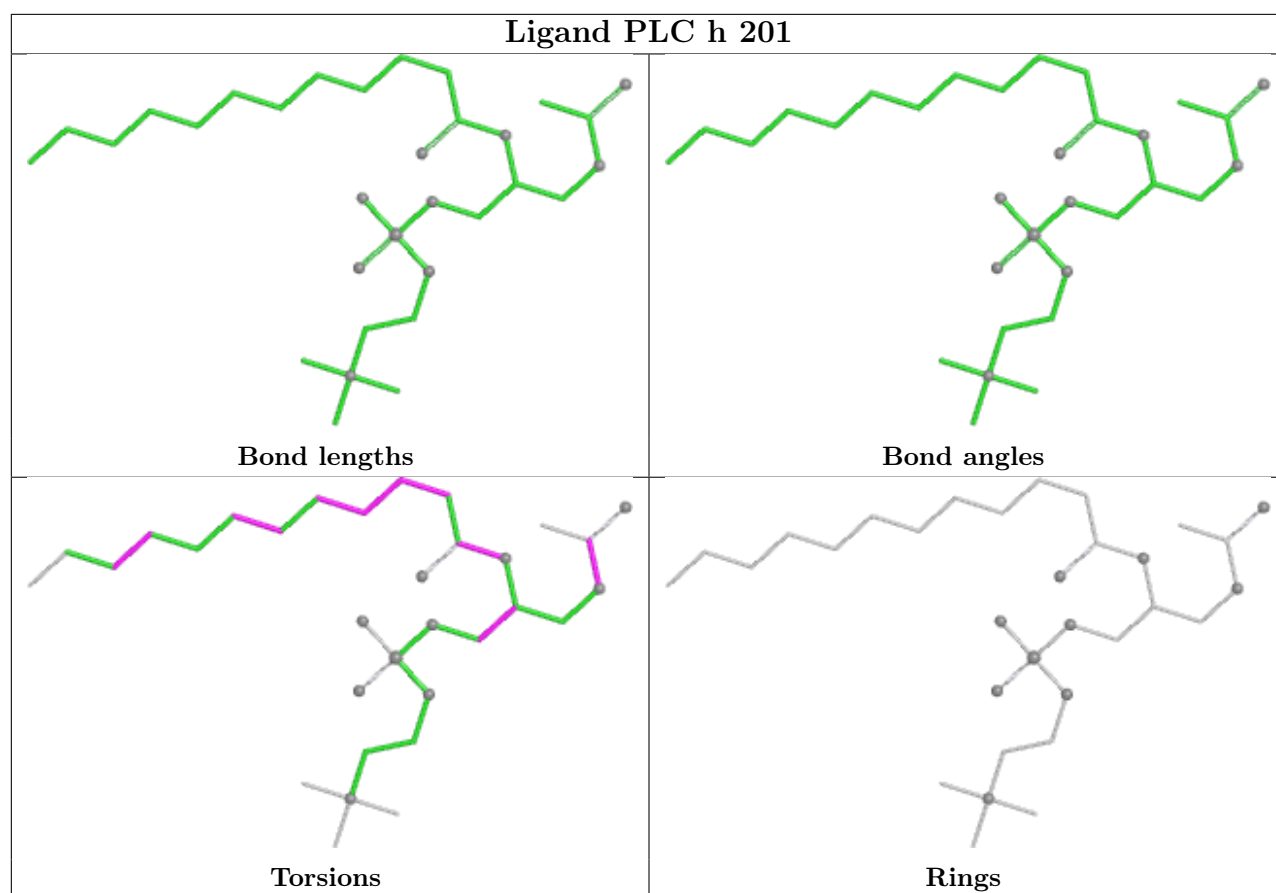


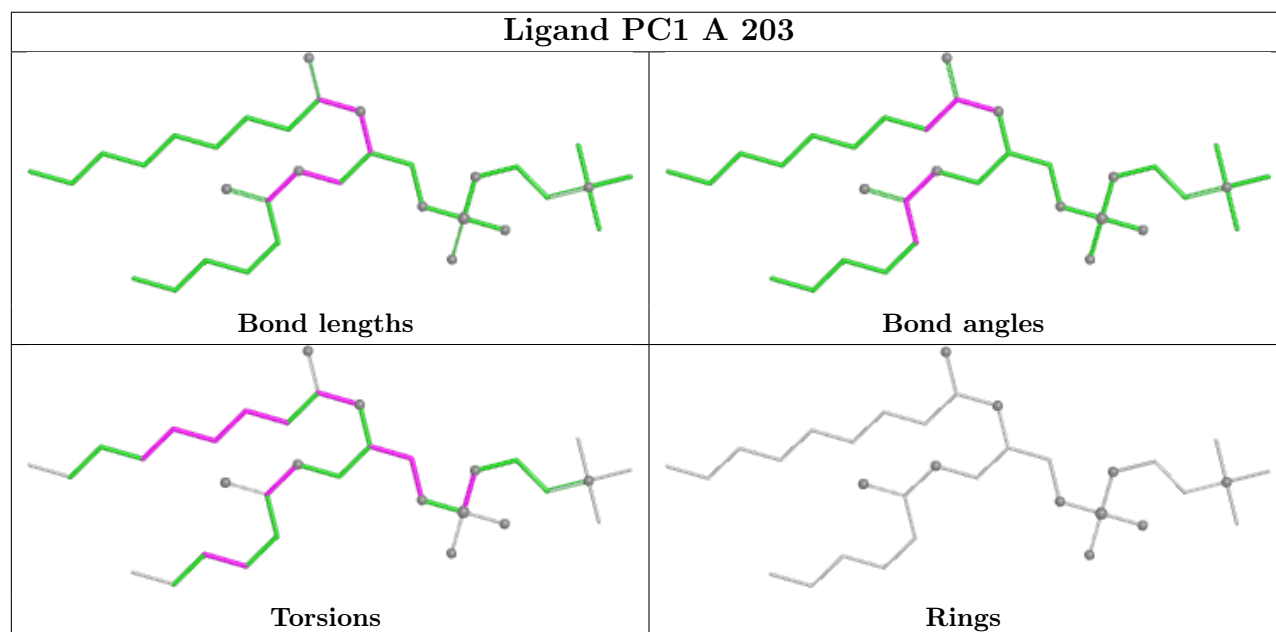
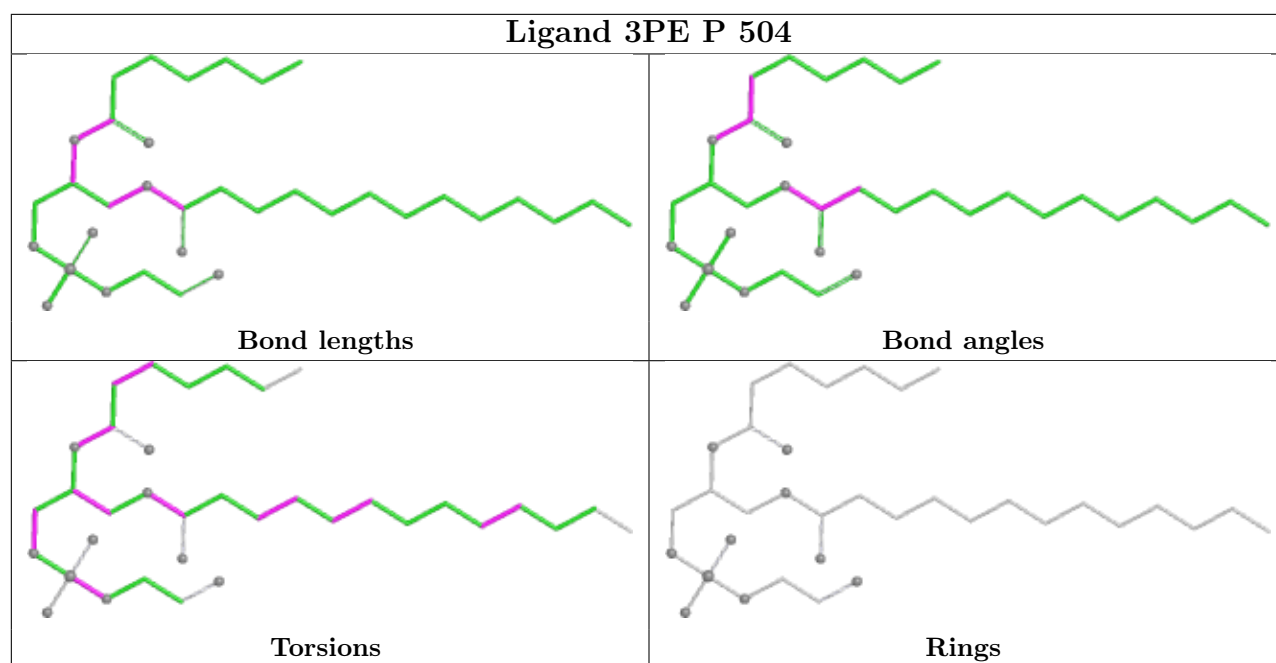


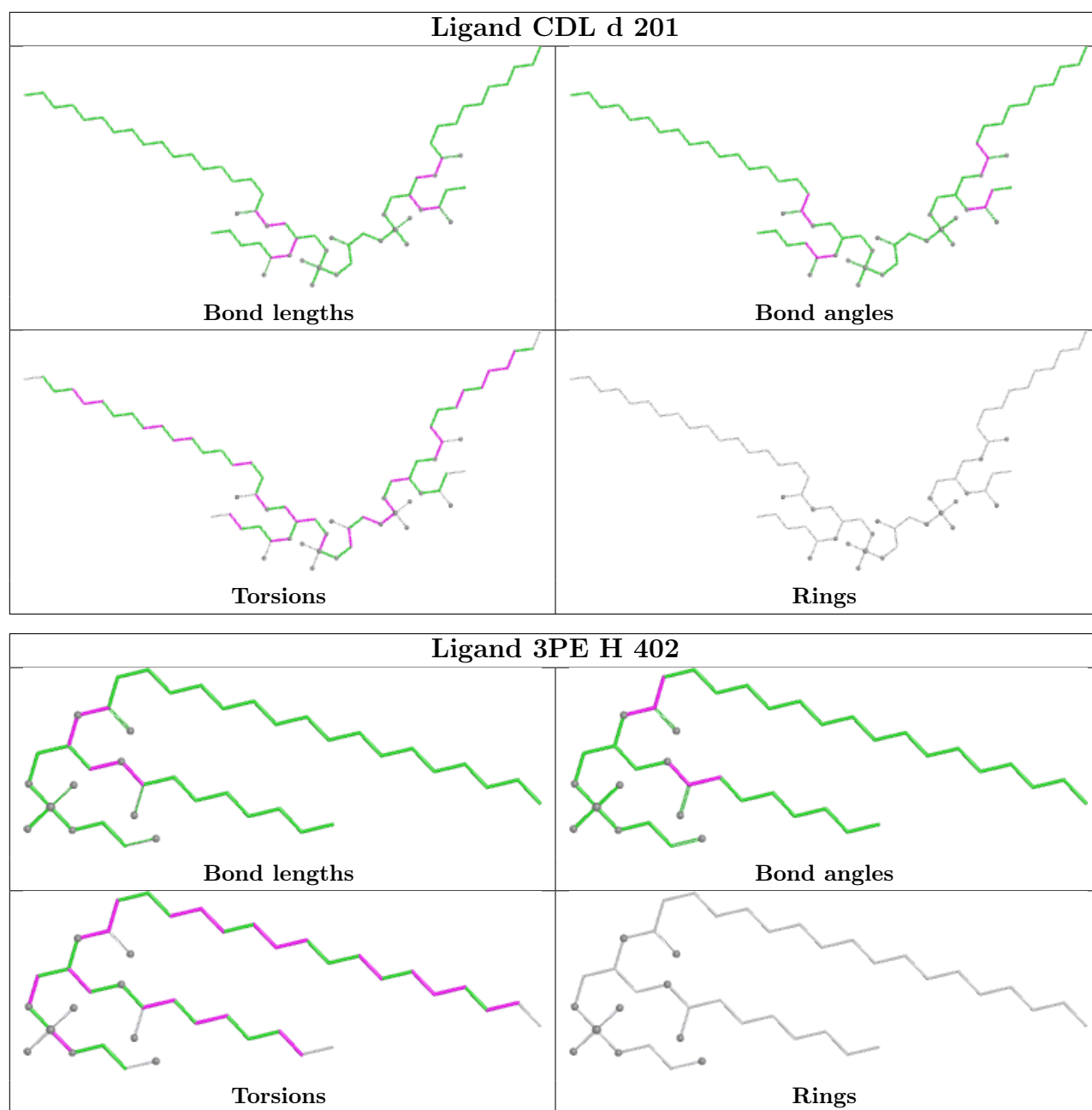


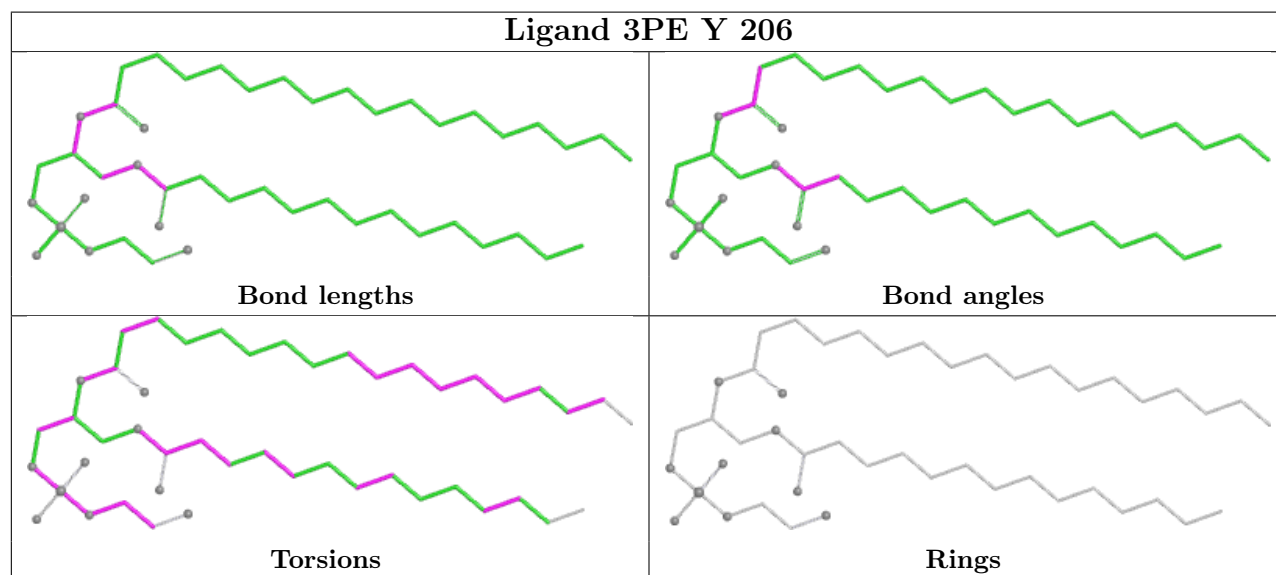
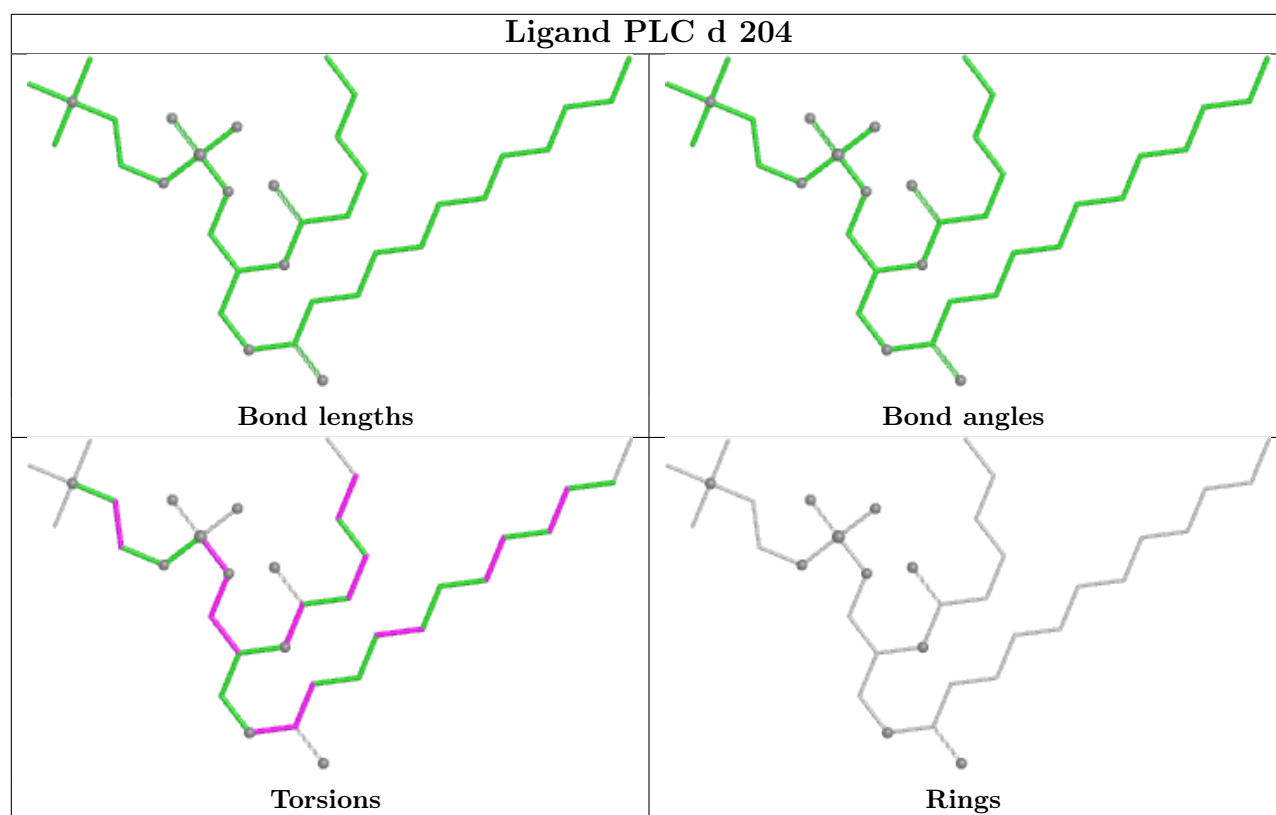


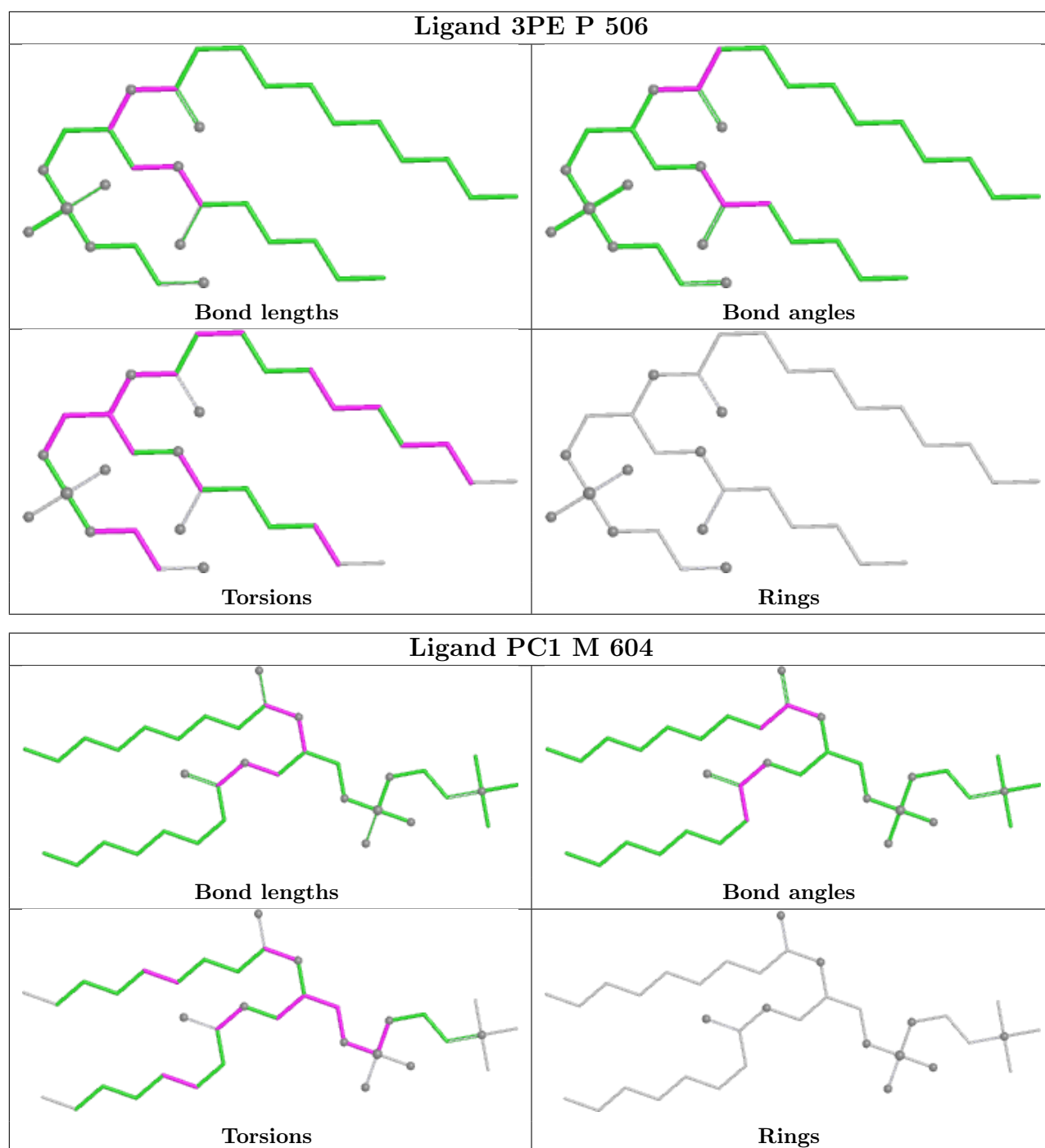


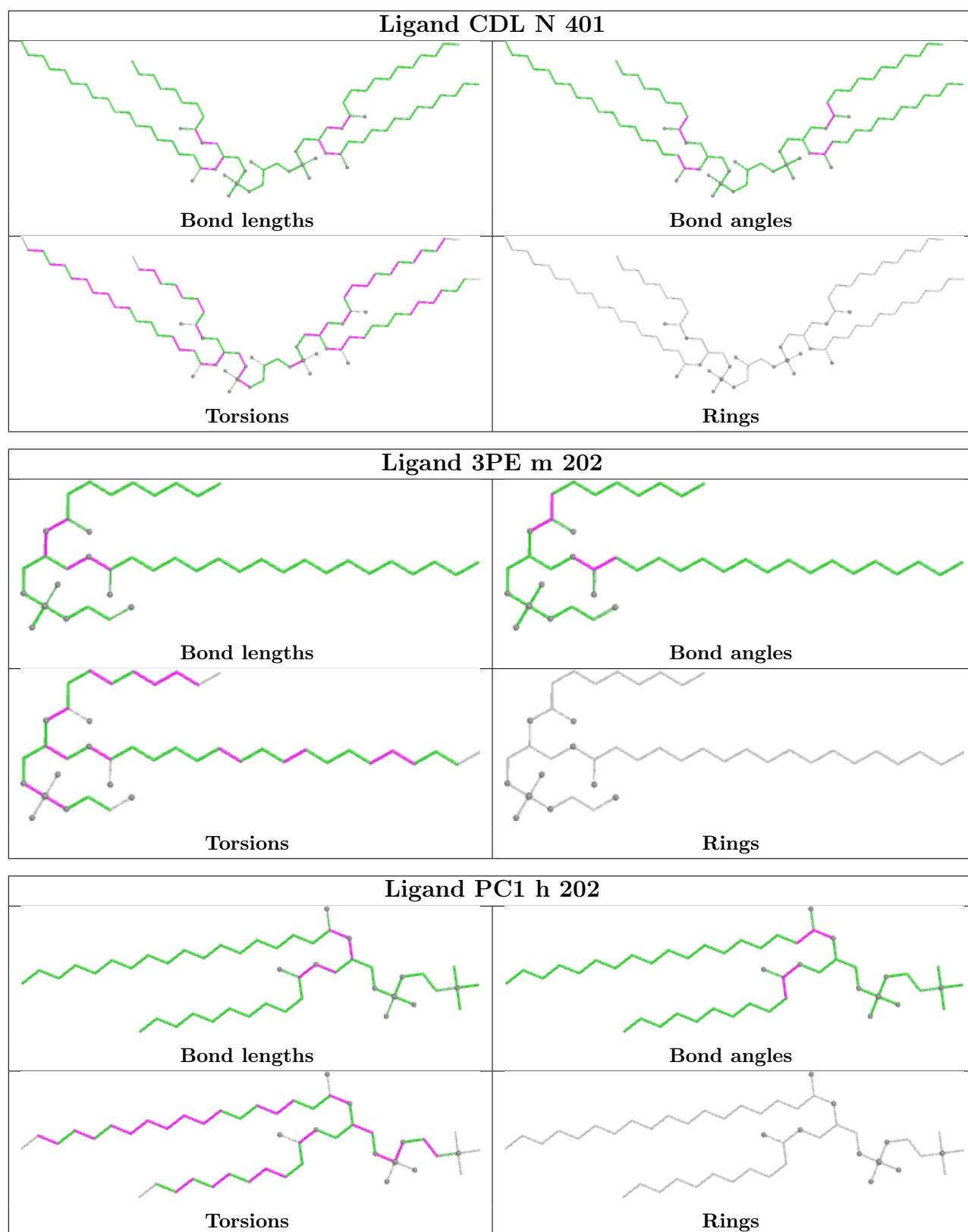


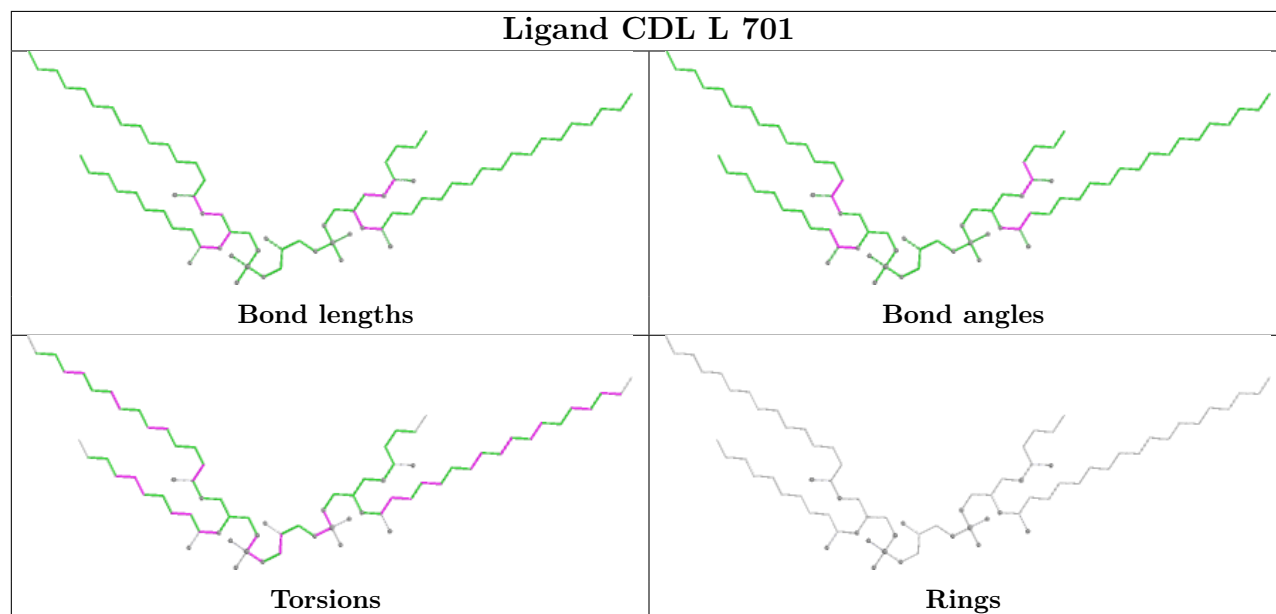
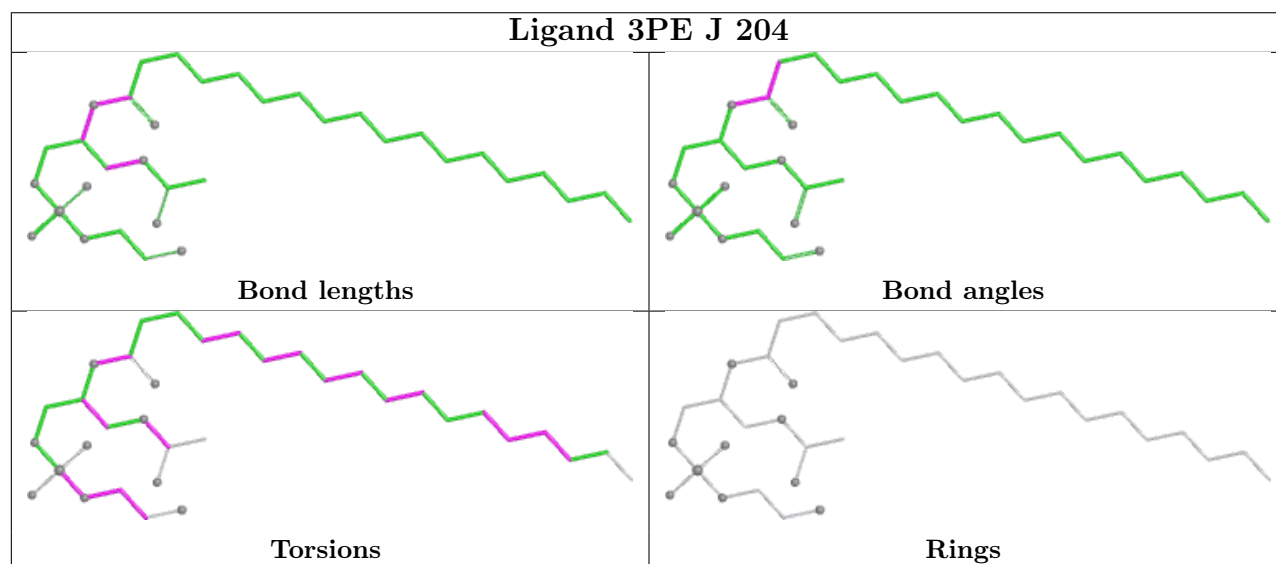
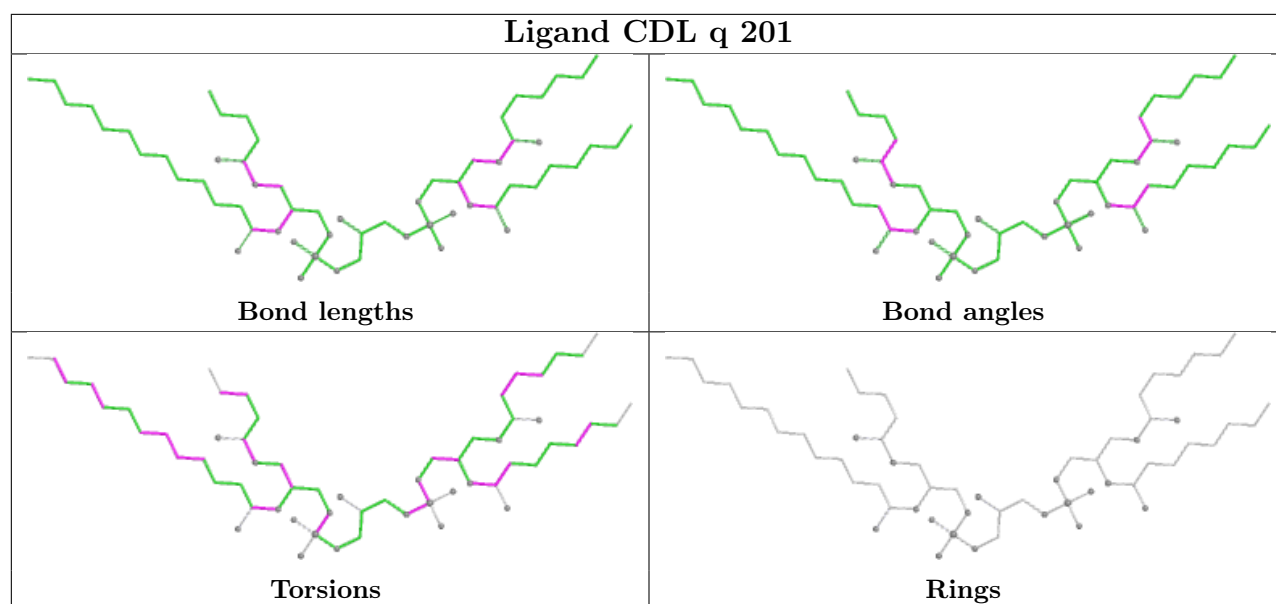


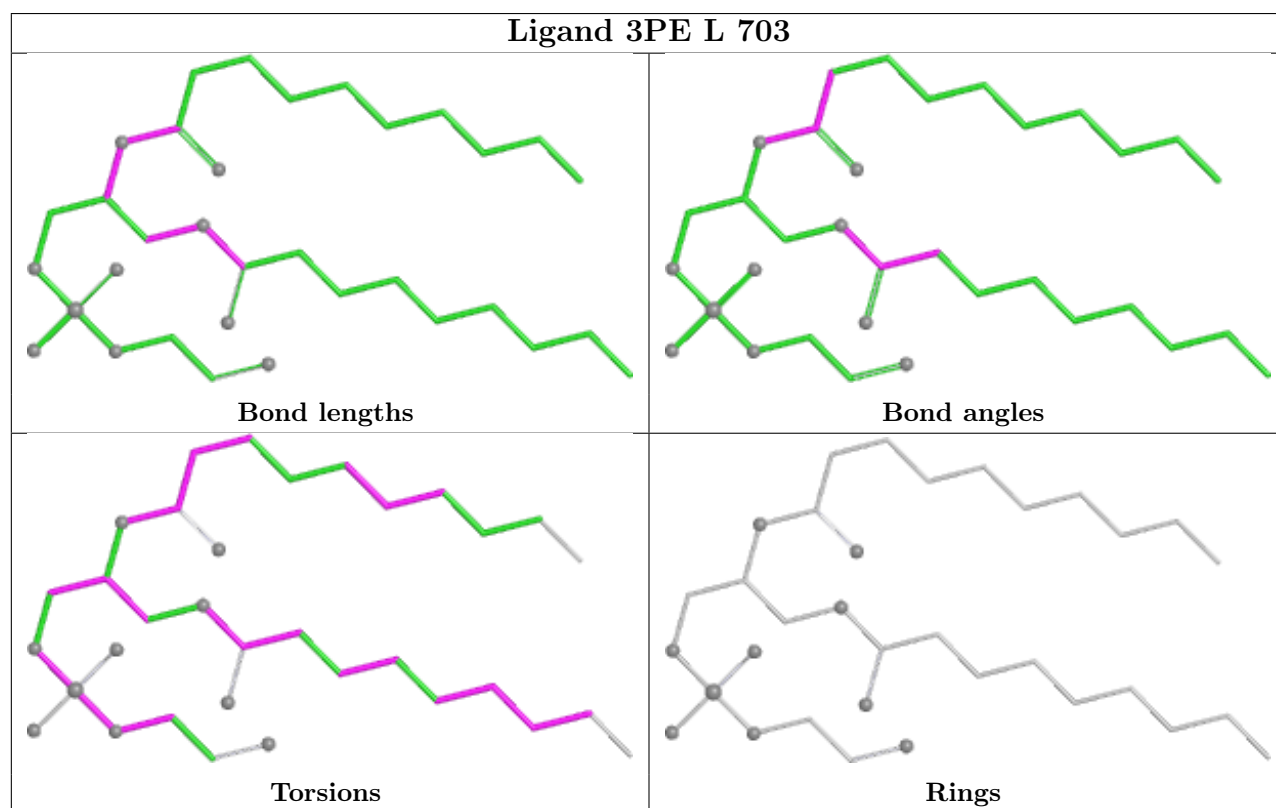
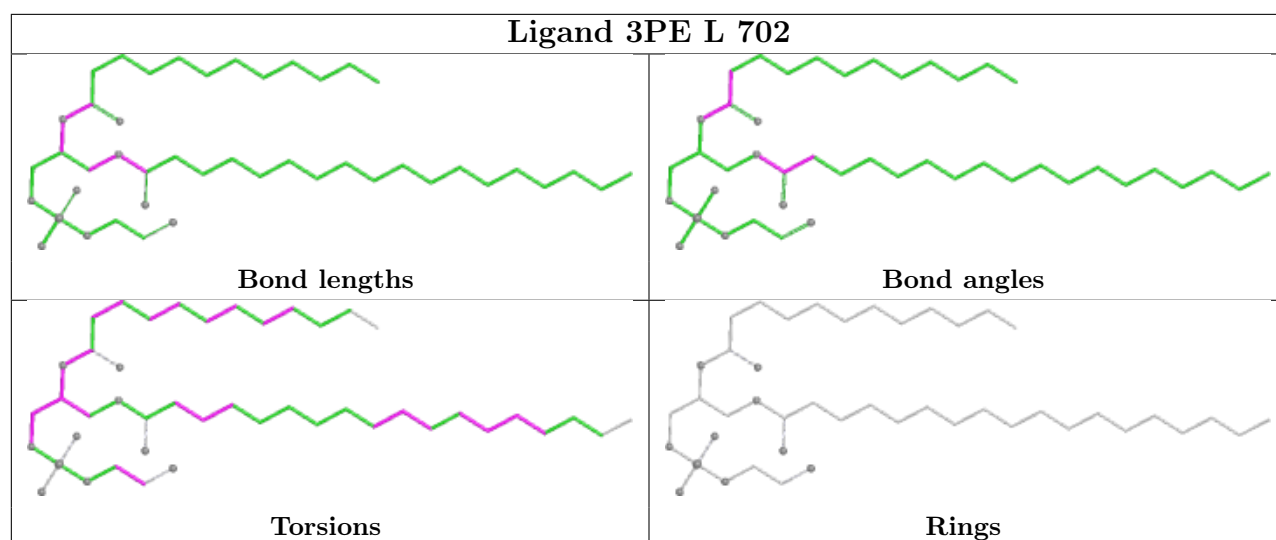


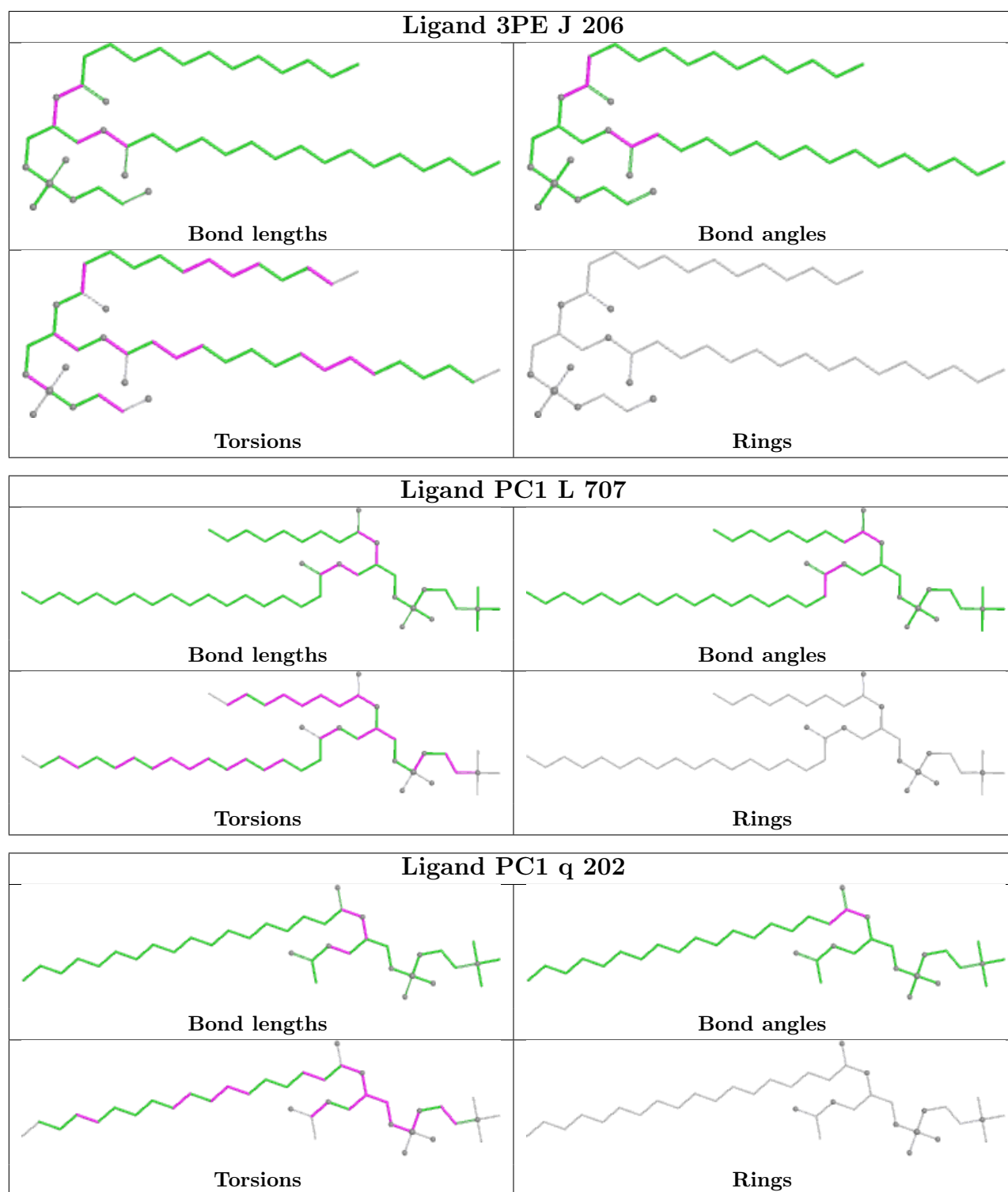


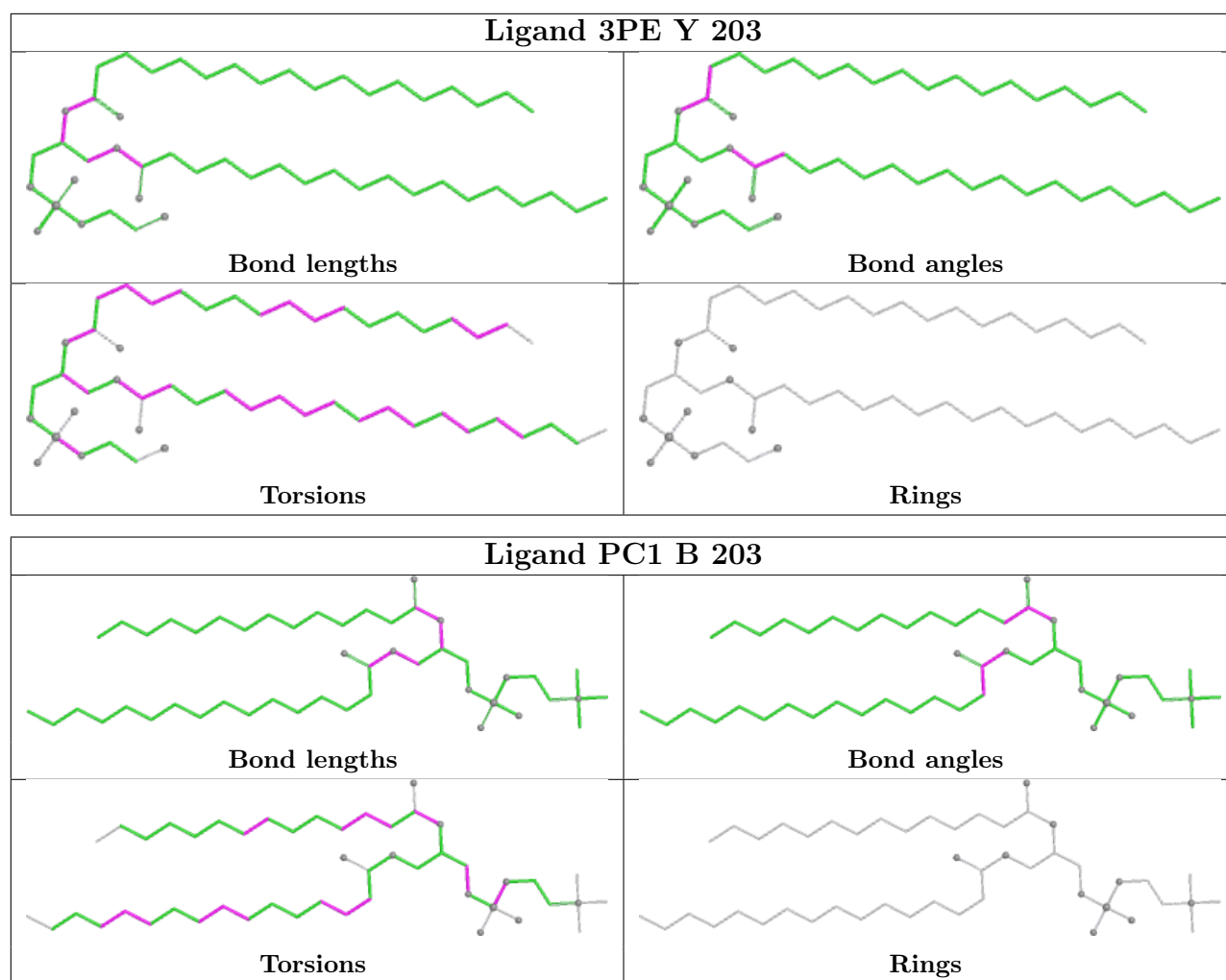


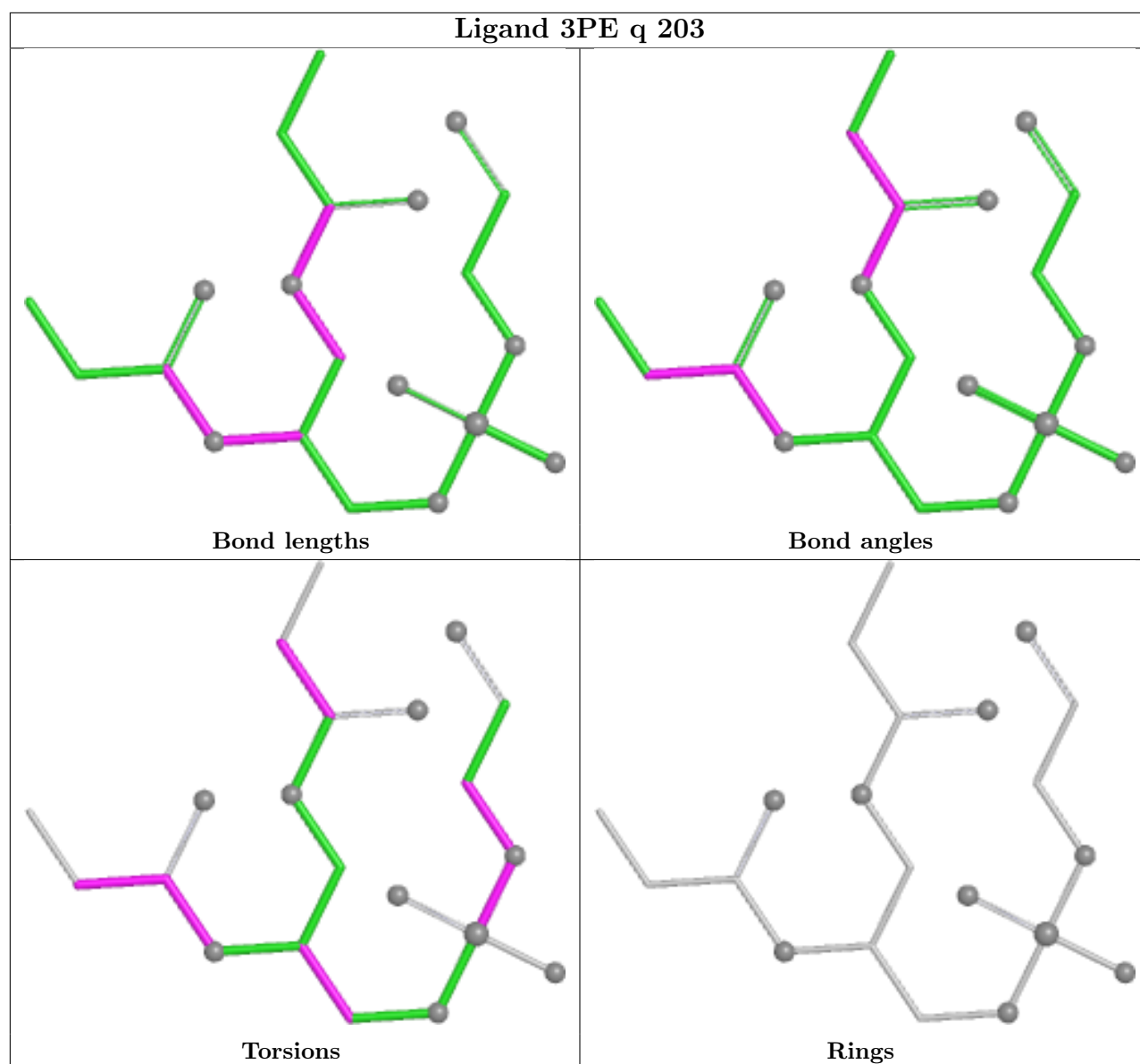


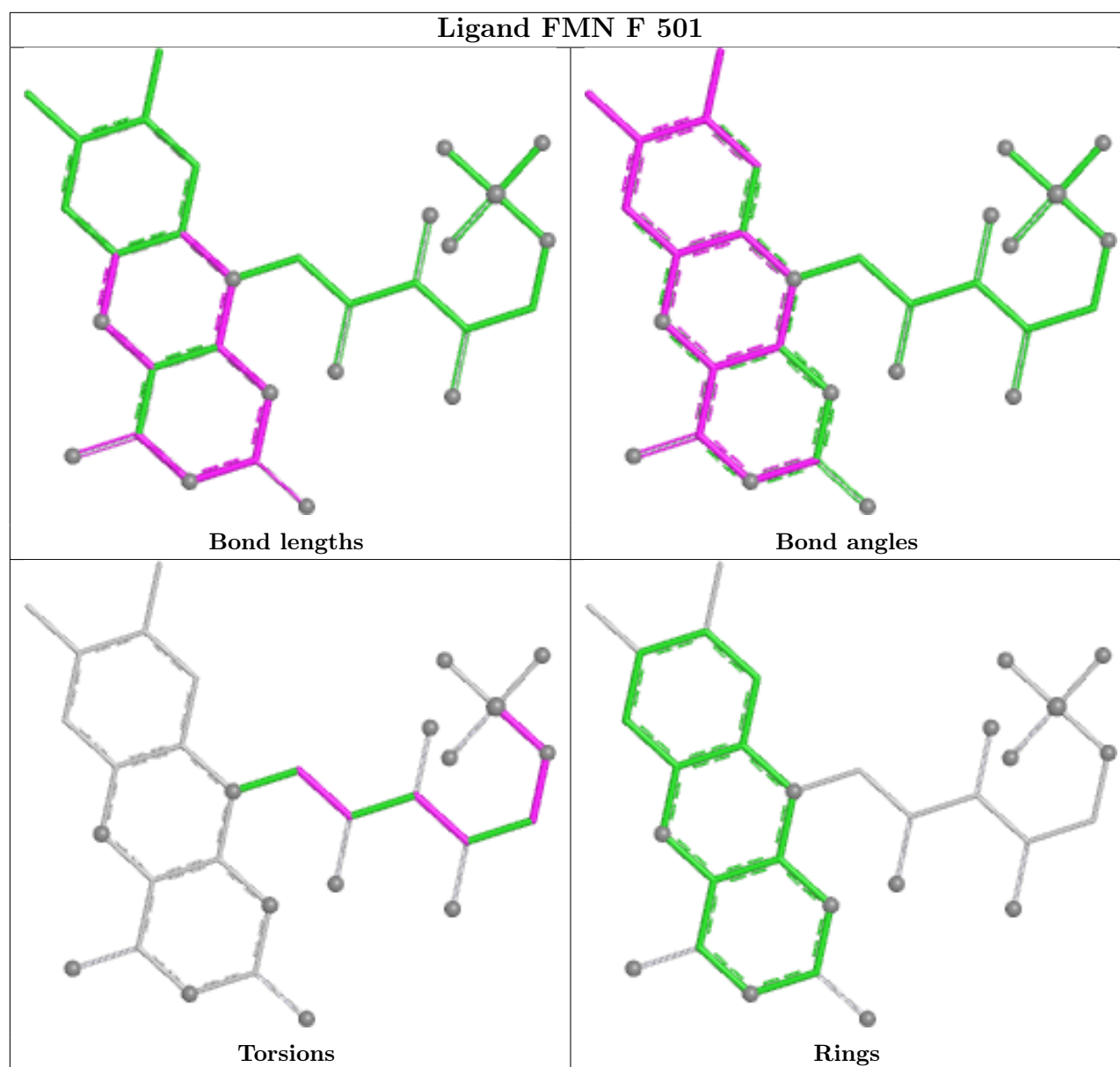












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

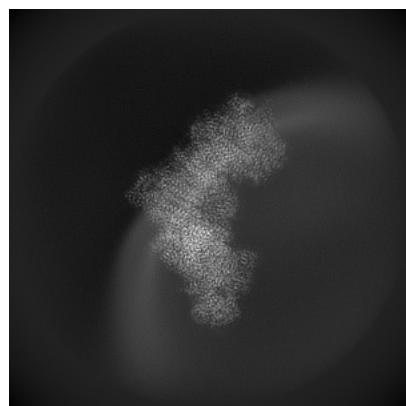
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18138. These allow visual inspection of the internal detail of the map and identification of artifacts.

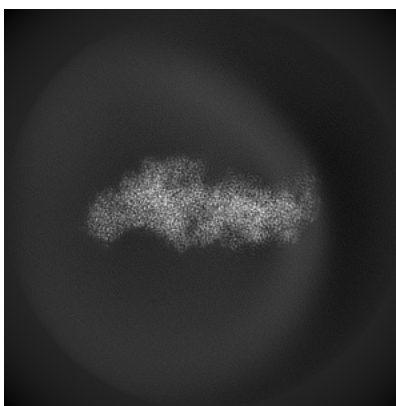
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

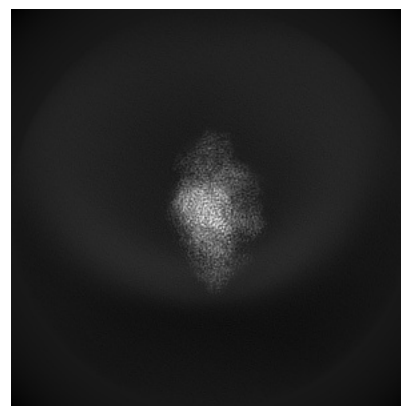
6.1.1 Primary map



X

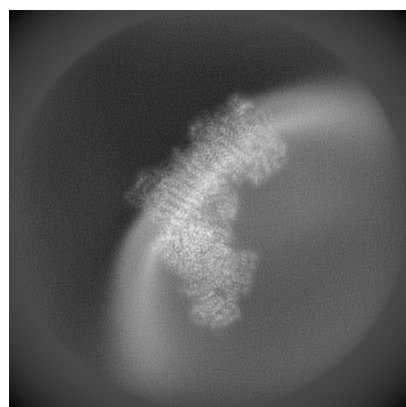


Y

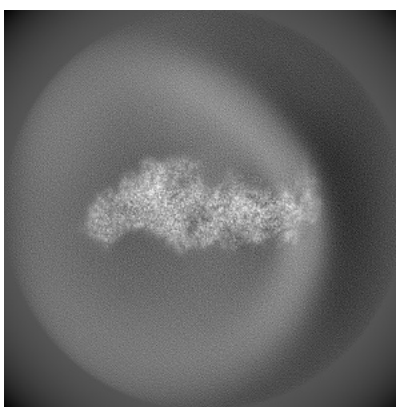


Z

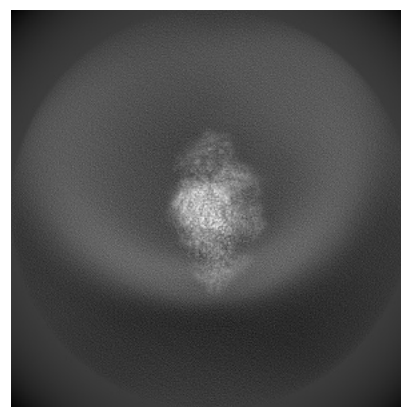
6.1.2 Raw map



X



Y



Z

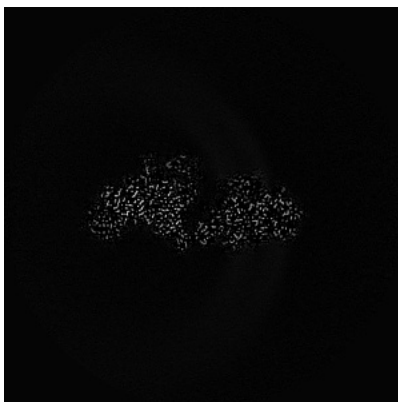
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

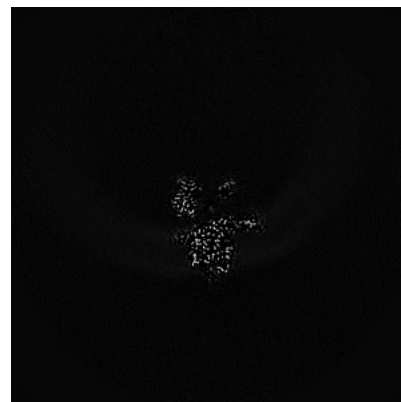
6.2.1 Primary map



X Index: 225

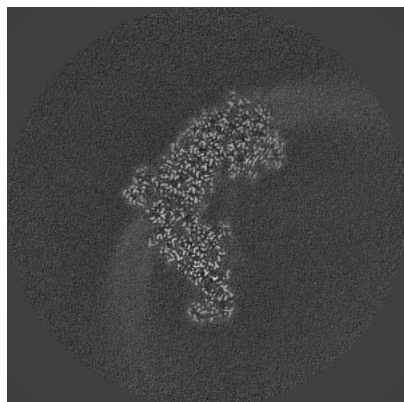


Y Index: 225

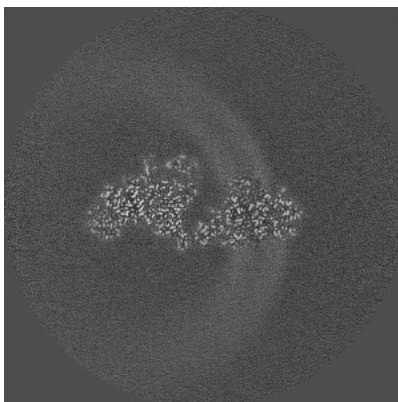


Z Index: 225

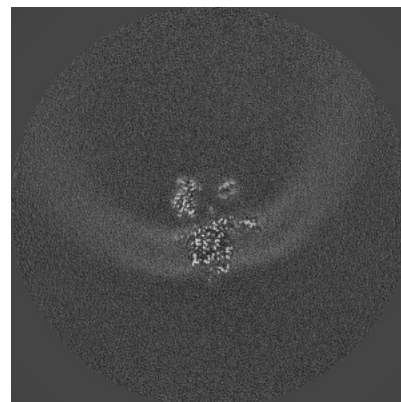
6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

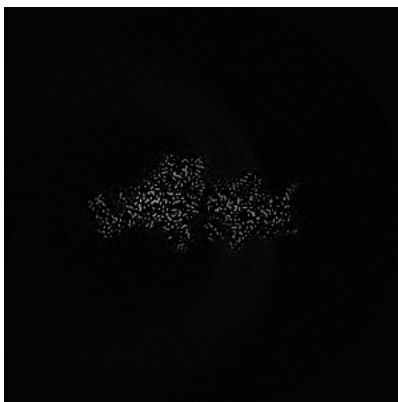
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

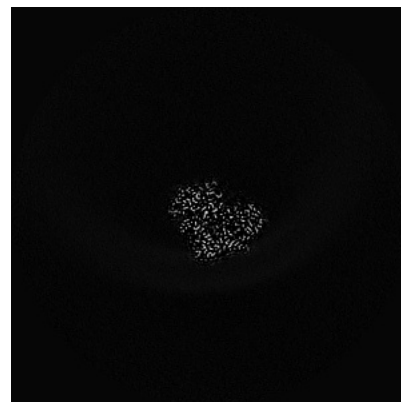
6.3.1 Primary map



X Index: 230

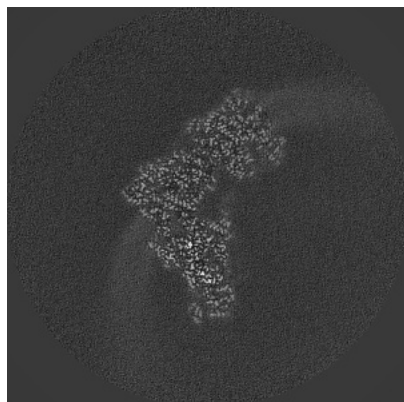


Y Index: 213

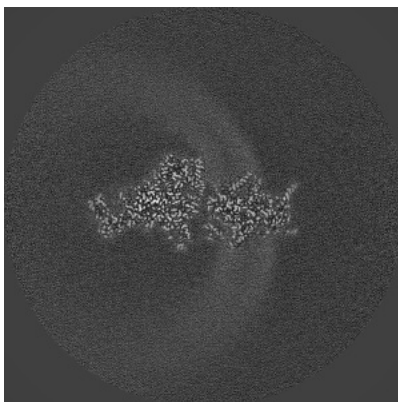


Z Index: 193

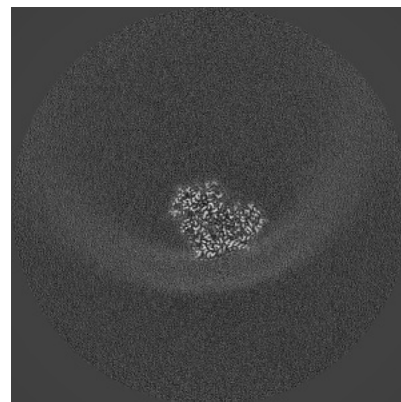
6.3.2 Raw map



X Index: 230



Y Index: 213

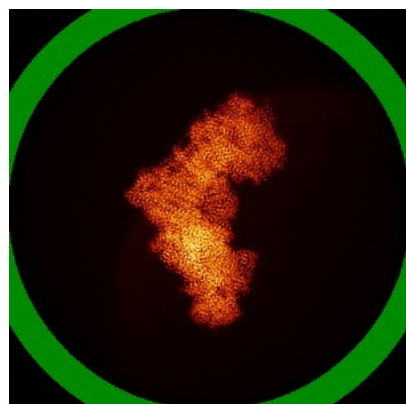


Z Index: 193

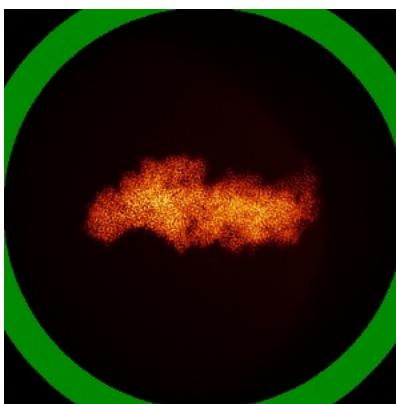
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

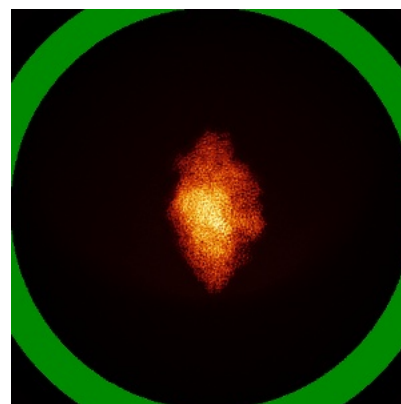
6.4.1 Primary map



X

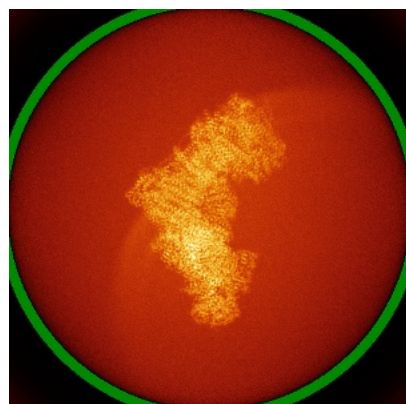


Y

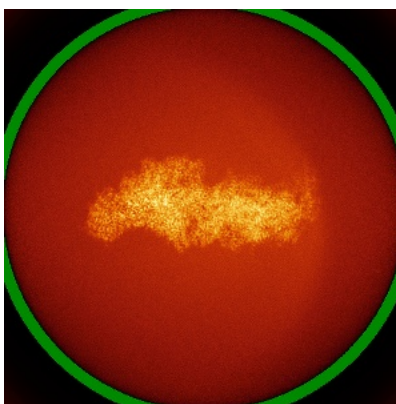


Z

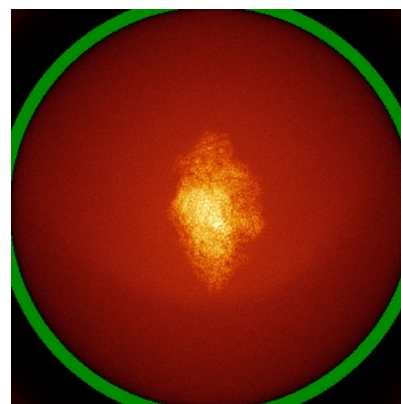
6.4.2 Raw map



X



Y



Z

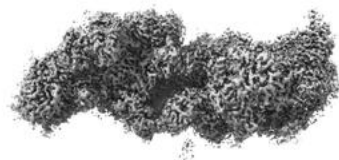
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

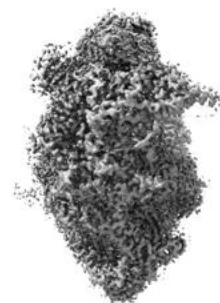
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

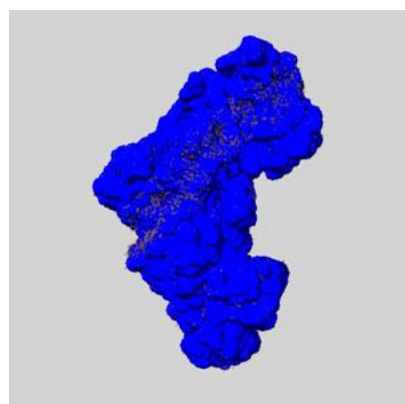
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

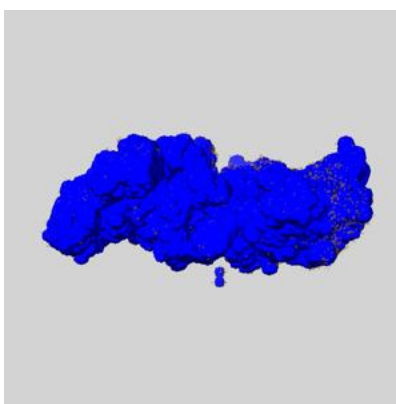
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

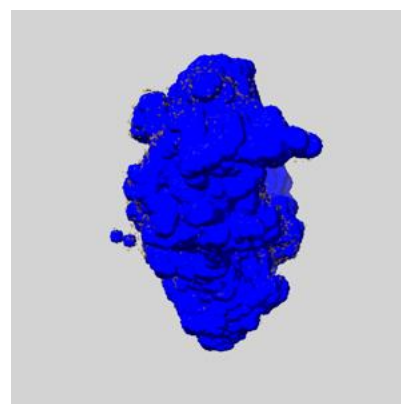
6.6.1 emd_18138_msk_1.map [i](#)



X



Y

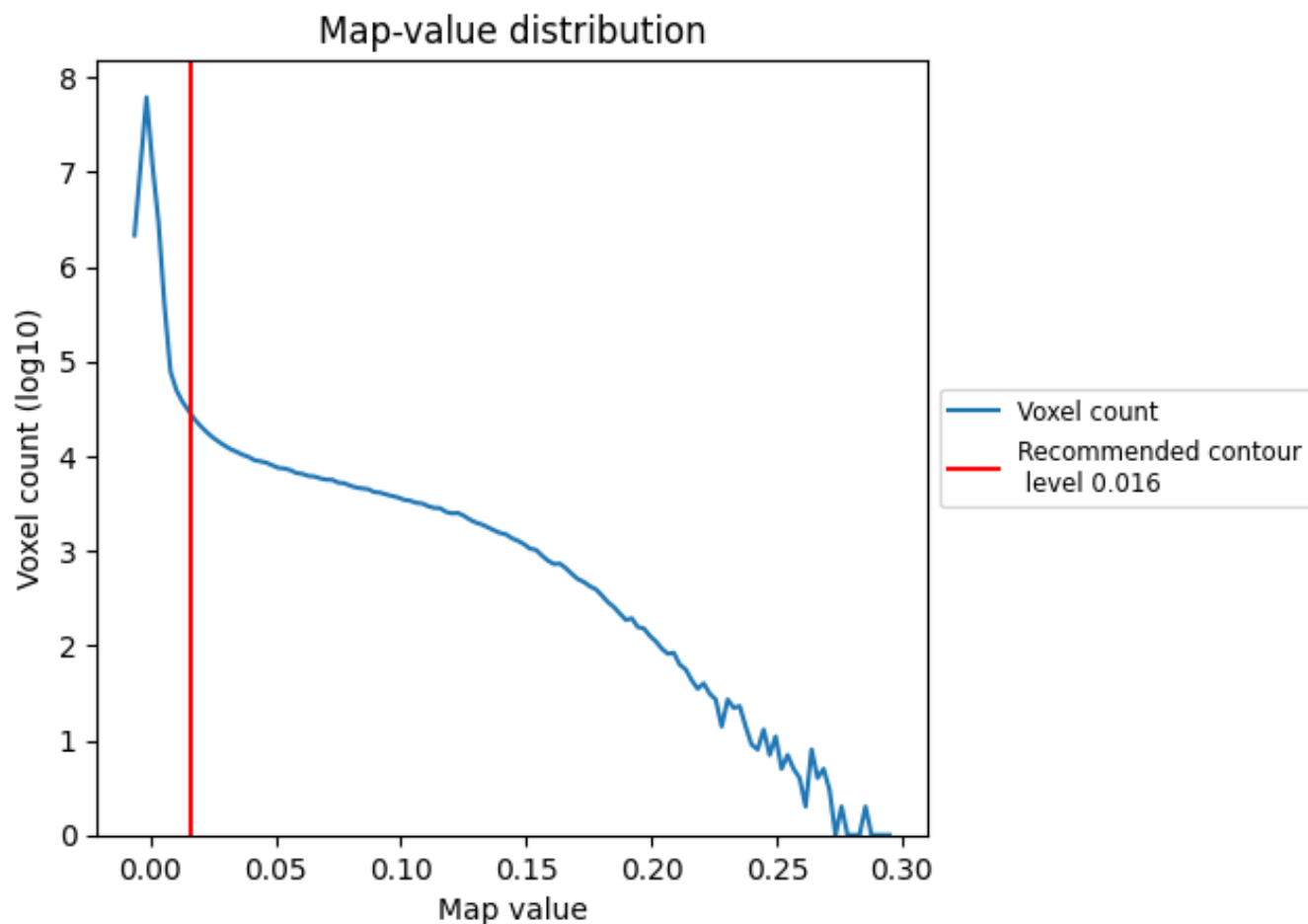


Z

7 Map analysis [i](#)

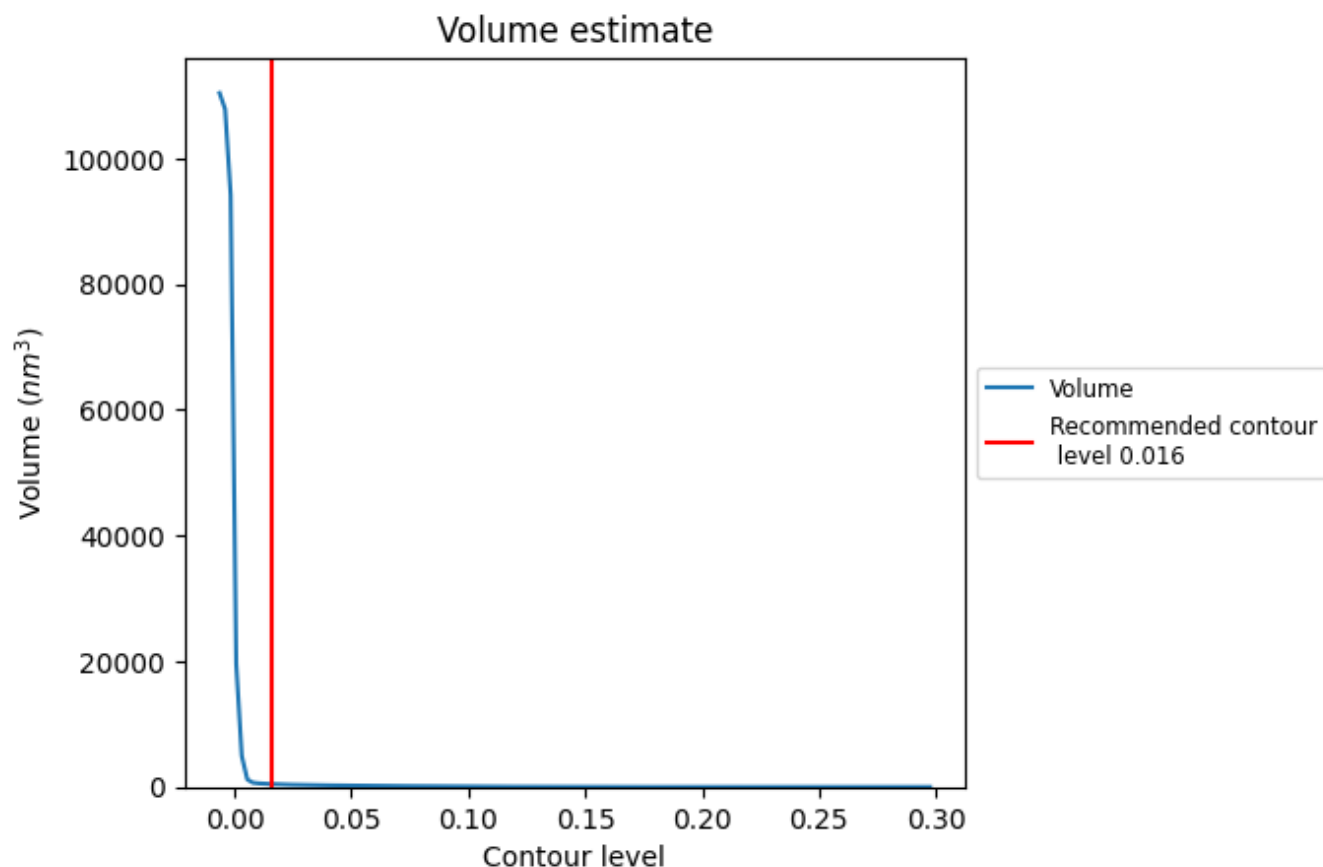
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

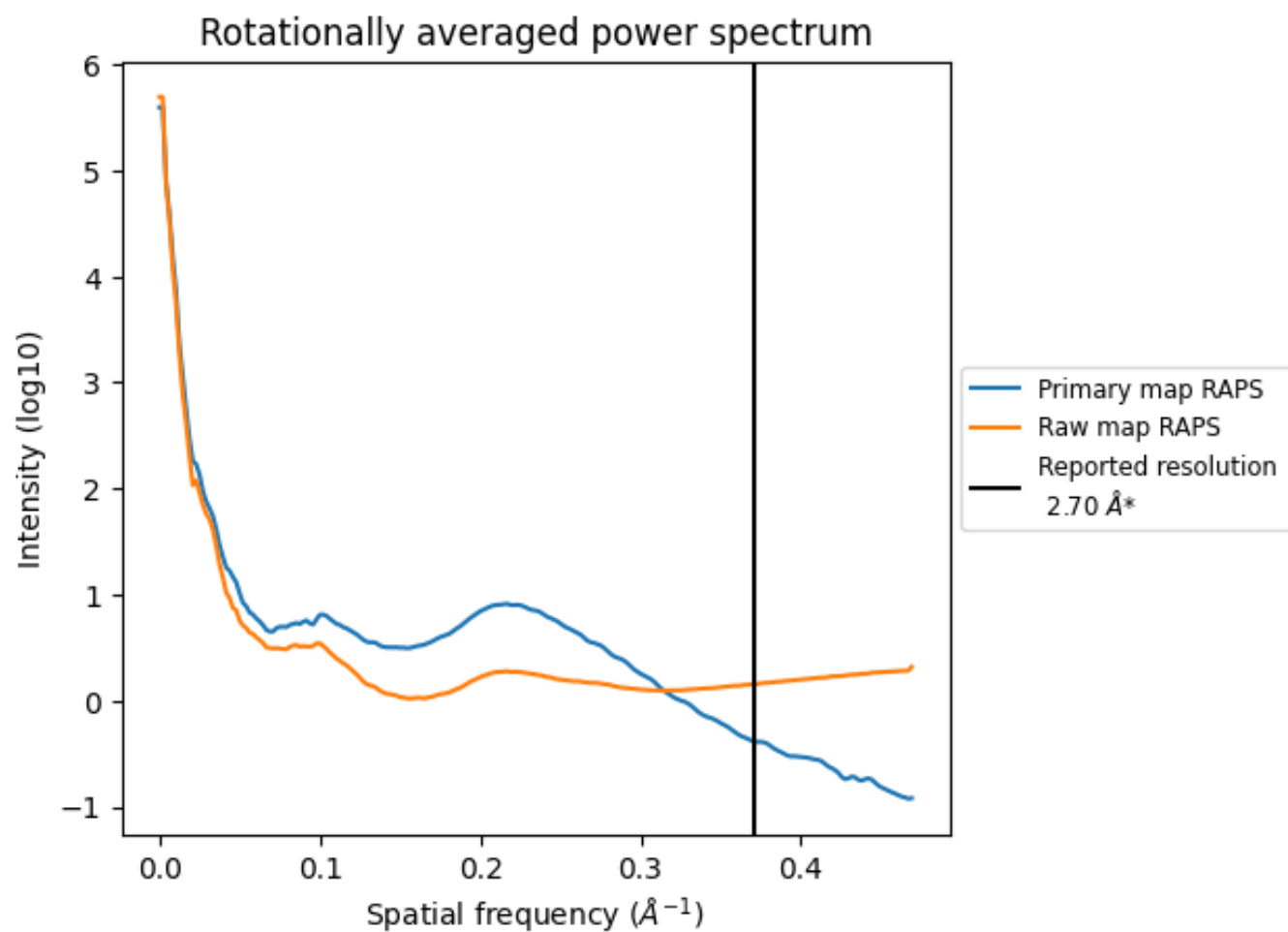
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 457 nm^3 ; this corresponds to an approximate mass of 413 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

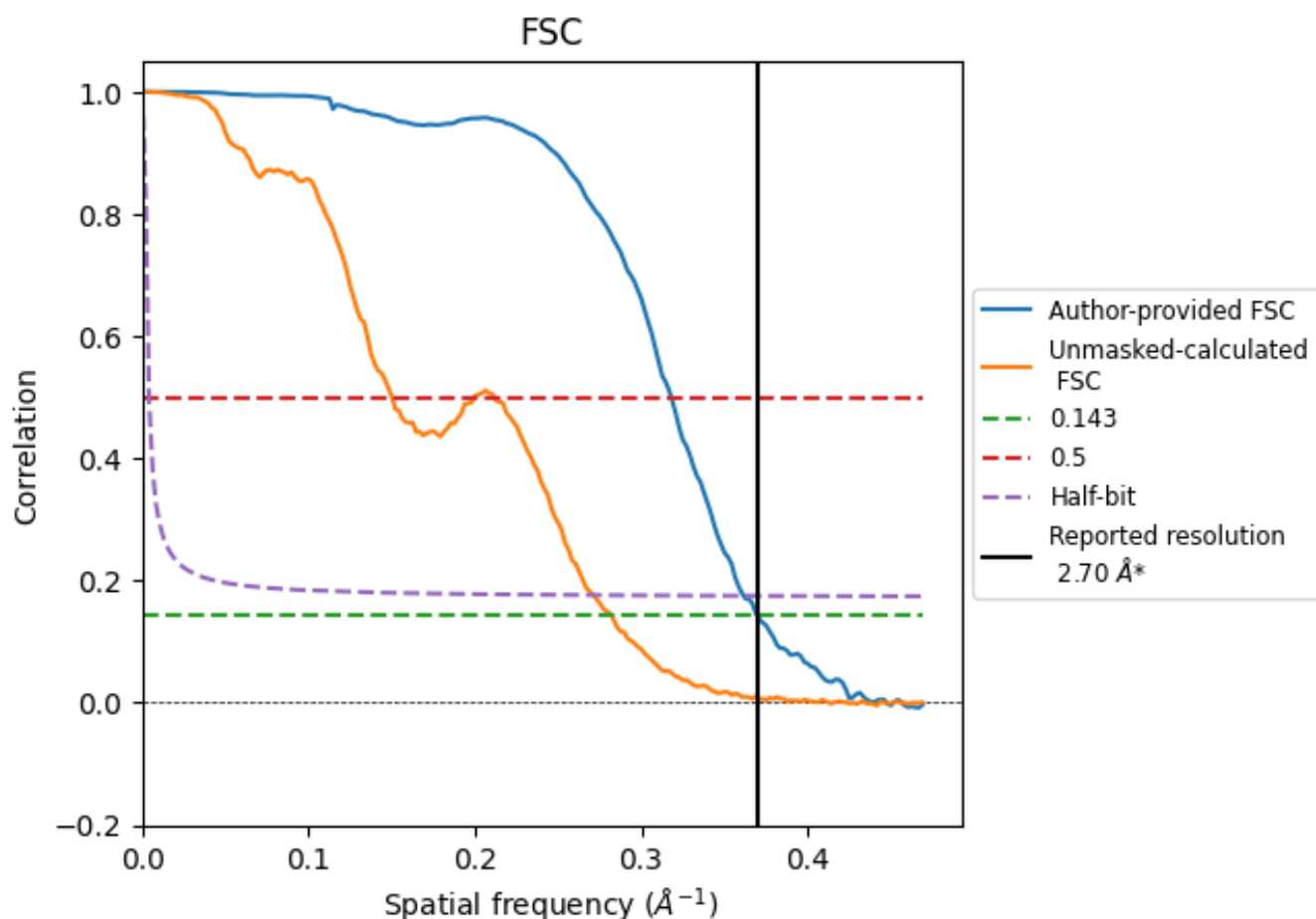


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

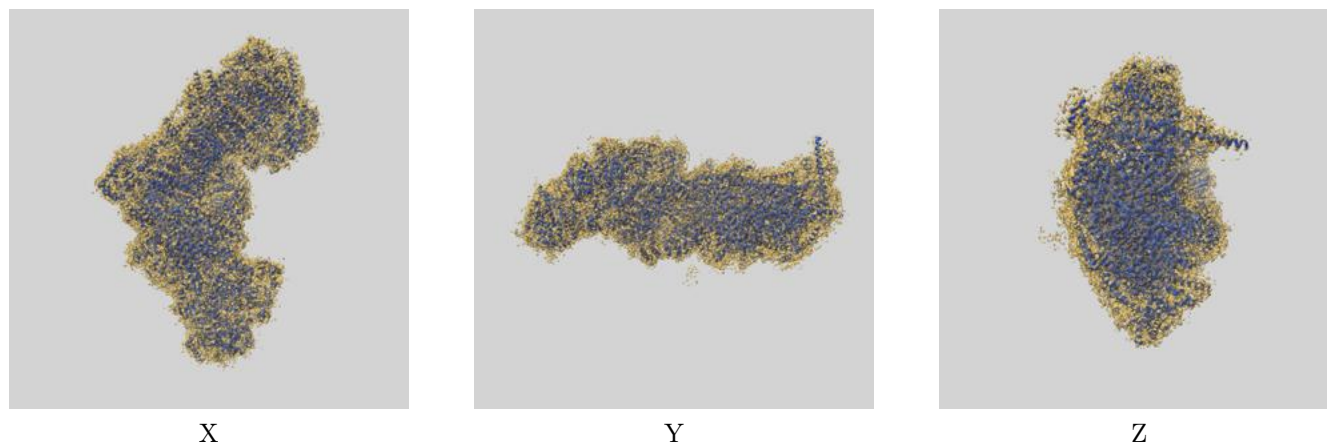
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.14	2.76
Unmasked-calculated*	3.55	6.66	3.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

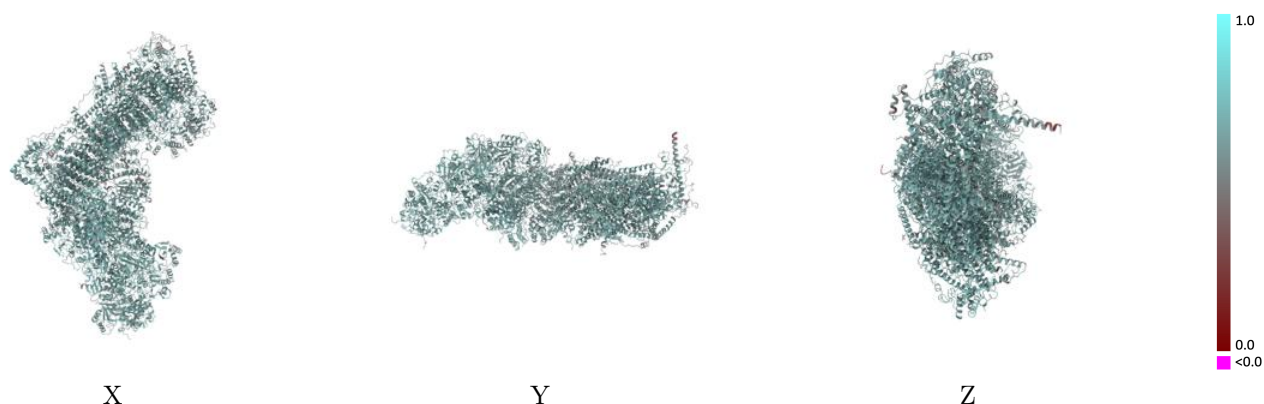
This section contains information regarding the fit between EMDB map EMD-18138 and PDB model 8Q45. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



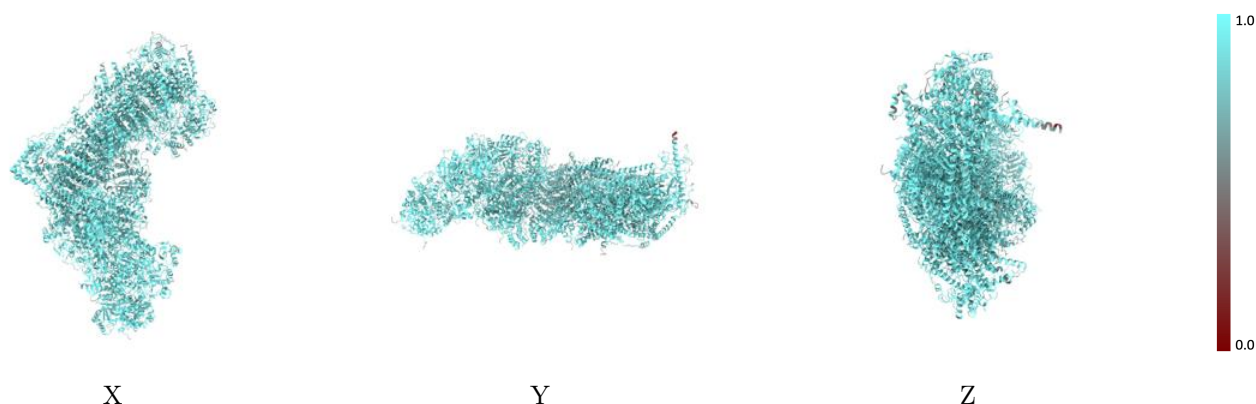
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



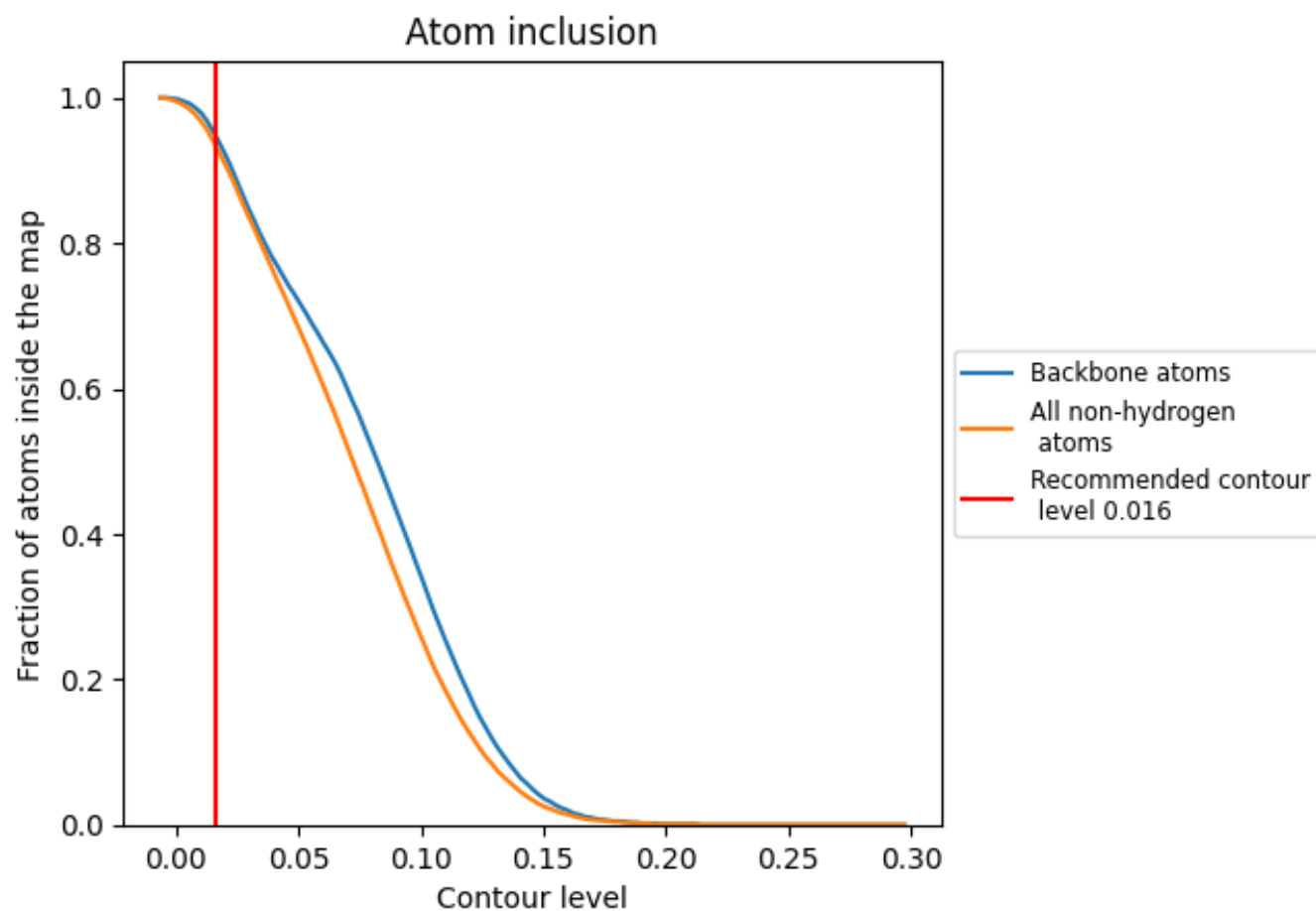
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9350	 0.6330
A	 0.9410	 0.6420
B	 0.9710	 0.6620
C	 0.9730	 0.6650
D	 0.9610	 0.6600
E	 0.9340	 0.6230
F	 0.9460	 0.6390
G	 0.9500	 0.6430
H	 0.9700	 0.6560
I	 0.9720	 0.6680
J	 0.9390	 0.6300
K	 0.9620	 0.6470
L	 0.9340	 0.6260
M	 0.9690	 0.6520
N	 0.9810	 0.6610
O	 0.9420	 0.6300
P	 0.9430	 0.6370
Q	 0.9490	 0.6440
R	 0.9450	 0.6490
S	 0.8820	 0.5970
T	 0.8200	 0.5540
U	 0.8710	 0.5830
V	 0.9500	 0.6480
W	 0.9490	 0.6450
X	 0.9250	 0.6250
Y	 0.8990	 0.6120
Z	 0.9390	 0.6330
a	 0.9520	 0.6470
b	 0.9200	 0.6230
c	 0.8960	 0.6090
d	 0.9190	 0.6270
e	 0.9090	 0.6180
f	 0.8310	 0.5750
g	 0.9040	 0.6140
h	 0.9580	 0.6400



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.8510	 0.5700
j	 0.8310	 0.5880
k	 0.8260	 0.5570
l	 0.9130	 0.6150
m	 0.8850	 0.6110
n	 0.9000	 0.6050
o	 0.8460	 0.5760
p	 0.8960	 0.6090
q	 0.9340	 0.6390
r	 0.9570	 0.6470
s	 0.9190	 0.6150